PARAMETER ESTIMATION IN NONLINEAR DIFFUSION PROBLEMS BY AN INVERSE TECHNIQUE

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Certificate

It is certified that the work contained in the thesis entitled **Parameter Estimation in Nonlinear Diffusion Problems by an Inverse Technique** by Narugopal Ghata, has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

K Muralidhar

February, 2000

K. Muralidhar
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To
my mother

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Abstract

The present study is concerned with the determination of parametric functions in nonlinear diffusion-dominated differential equations by an inverse technique. Examples of these functions are thermal conductivity and heat capacity in a conduction problem and relative permeability and capillary pressure in flow through an unsaturated porous medium. The parameters to be estimated are embedded in a partial differential equation and are constrained by the physical laws of nature. Hence it is to be expected that the objective function setup to estimate the parameters would be continuous and display monotone properties. The most appropriate optimization method technique needed to extract the parameters is then naturally based on gradient search. The conjugate gradient algorithm has been employed as the search technique in the present study. The gradient of the objective function requires the calculation of the adjoint of the differential operator governing the physical process. The use of the adjoint function makes the estimated parametric functions to be physically meaningful since the mirror image of the natural law is simultaneously enforced in the calculations.

The objective function has been constructed in the present work by comparing the discrete measured state variables with their values corresponding to assumed property functions. This leads to a correction formula for the properties when the objective function is minimized. Th1s procedure has been cast in the form of a computational algorithm. The algorithm is iterative in nature and is strated with reasonable initial guess.

Numerical results obtained in the present work show that the inverse procedure is capable of reasonable predictions of the unknown parameters. Larger errors are seen under certain conditions for small time and points located close to the boundaries. Errors are also observed when the process approaches the steady state. The reconstruction of the parameters is generally found to be sensitive to random errors in the measurement data.

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Nomenclature

[All quantities reffered are dimensionless, unless otherwise specified]

$C(T)$ or $C(x,t)$	Heat capacity
J	Objective function
J'	Gradient of the objective function
$K(T)$ or $K(x,t)$	Thermal conductivity
L	Vector operator of the governing differential equations
L_{UB}	Vector operator representing upper boundary conditions
L_{LB}	Vector operator representing lower boundary conditions
M	Number of sensors used to measure the state variables
P	Direction of descent in the optimization problem
S	Sensitivity
T	Estimated dimensionless temperature
ΔT	Sensitivity function
Y	Measured temperature
p	Column matrix of unknown paramters
u	Column matrix of state variables
Greek Symbols	
β	Search step size
ν	Conjugate coefficient
δ	Dirac Delta function
$\lambda(x,t)$	Lagrange multiplier or Adjoint function
ω	Random number
Superscript	
$-$	Dimensional parameters
n	Iteration index
Subscript	
r	Reference parameter

Chapter 1

Introduction

When a numerical model is used to simulate a practical problem, the parameters which appear in terms of coefficients and/or initial and boundary conditions of the governing equation must be specified. The parameters are not directly measurable from the physical point-of-view. The inverse approach provides a way wherein measurements of state variables are used to determine the unknown parameters. (This may include the unknown initial or boundary conditions). In the inverse problem of function estimation, one can guess the values of the parameters. Then by minimizing the differences between estimated and experimental values of the state variables the required parameters can be estimated. Therefore, the inverse problem can be formulated as an optimization problem.

Numerical solution of the optimization problem can be classified into the following three categories: Gauss-Newton, gradient search, and direct search methods. In order to obtain the Gauss-Newton direction it is necessary to calculate the sensitivity matrix in each iteration of the nonlinear least squares method. If a gradient search method is used to solve the optimization problem, it is necessary to calculate the gradient vectors during each iteration. Gradient search methods are designed to avoid the calculation of the sensitivity matrix. Therefore, in principle, they require less computer time. However, more iterations may be required for convergence. Direct search methods do not require the calculation of either the sensitivity matrix or the gradient vector. However, the rate of convergence of such methods is generally slow.

Gradient search methods have been used during optimization encountered in the inverse problem. During the past two decades, there has been great interest in the use of

the conjugate gradient method in iterative minimization procedures applied to the solution of constrained and unconstrained problems involving linear and nonlinear equations. Very recently, the method has been applied to the solution of the inverse problem. The commonly used gradient search method utilizes the direction of negative gradient of the functional as the search direction, while the conjugate gradient method uses a combination of the negative gradient of the functional and the previous descent directions for search. Obviously, methods that calculate each new direction of search as a part of the descent direction at the last iteration are inherently more powerful than those in which the directions are assigned in advance.

1.1 Importance of the Problem

Thermal properties such as thermal conductivity and heat capacity play an important role in the transport of heat in a wide variety of materials. This can be gauged by the fact that a property like thermal conductivity can vary over six orders of magnitudes in commonly encountered materials, and upto ten orders in certain cases. Over and above the large variation that is seen from one material to another, thermal properties also depend on temperature and composition. Thus, in a practical application, they can vary from point to point as well as with time.

Experimental determination of thermal properties as a function of temperature is a topic of great importance. Conventional methods for obtaining thermal properties include steady state, periodic heating, step response and pulse inputs. A majority of these methods utilize the constant property assumption. The data reduction process then reduces to a least squares procedure employing the error between the estimated and measured temperatures.

In many applications, the parameters to be estimated may change with position, time or the dependent variables themselves. A prominent example is establishing the constitutive relations for multiphase flow in a porous media. For example, the parameters appearing in oil-water flow through a porous formation are relative permeability of oil, relative permeability of water, capillary pressure and porosity. Porosity can be assumed to be constant for a homogeneous medium. Relative permeability of oil and water are functions of water saturation. Water saturation is also a function of capillary pressure,

namely the difference between oil and and water phase pressures. Modeling of these relationships is extremely important for oil reservoir simulation. The inverse approach provides a systematic route for determination of these constitutive relationships.

1.2 Literature survey

A survey of the literature reveals that various aspect of the inverse technique have been addressed. These have been presented below as per the following sections:

1.2.1 Uniqueness

The inverse problem is often ill-posed. The ill-posedness is characterized by the nonuniqueness and extensive dependence on data of the identified parameters. The latter stems from the fact that small experimental scatter will cause serious errors in the identified parameters.

Chavent [1974] studied the uniqueness problem in connection with parameter identification in distributed parameter systems. In the case of non-uniqueness, the identified parameters differ according to the initial estimate of the parameters, and there is no reason for the estimated parameters to be close to the "true" values. As a consequence, the responses of the model and the system will differ for inputs other than those that have been used for identification. Chavent studied the uniqueness problem for two situations: (1) the case of constant parameters and (2) the case of distributed parameters in space. In case 1, i.e., constant parameters, there are generally more measurements than unknowns. This forces the inverse problem to be unique in the sense of least squares. In case 2, i.e., distributed parameters, if only point measurements are available, the inverse problem is always nonunique. The term, point measurements refers to the situation where measurements are made only at a limited number of locations in the spatial domain.

The uniqueness problem in parameter estimation is intimately related to identifiability. The notion of identifiability addresses the question of whether it is all possible to obtain unique solutions of the inverse problem for unknown parameters of interest in a mathematical model, from data collected in the spatial and time domains. *Kitamura*

and Nakagiri [1977] formulated the parameter identification problem as the one-to-one property of the inverse problem, i.e., the one-to-one property of mapping from the space of system outputs to the space of parameters. However, the uniqueness of such a mapping is extremely difficult to establish and often nonexistent. The authors defined the identifiability as follows: "We shall call an unknown parameter "identifiable" if it can be determined uniquely in all points of its domain by using the input-output relation of the system and the input-output data." Kitamura and Nakagiri also obtained some results for parameter identifiability and nonidentifiability for a system characterized by linear, one-dimensional parabolic partial differential equation.

An independent definition of identifiability given by *Chavent* [1979*b*] is suited to the identification process using the output least square error criterion. The criterion used for solving the inverse problem of parameter identification is said to be output-least-square-identifiable if and only if a unique solution of the optimization problem exists and the solution depends continuously on the observations. Identifiability is usually not achievable in the case of point measurements where data is only available at a limited number of locations in the spatial domain.

1.2.2 Classification of Parameter Identification Methods

Various techniques have been developed to solve the inverse problem of parameter identification. Various methods of solving inverse heat conduction problems have been discussed by *Beck, Blackwell and Clair* [1985]. *Neuman* [1973] classified the techniques into either "direct" or "indirect." The "direct approach" treats the model parameters as dependent variables in a formal inverse boundary value problem. The "indirect approach" is based upon an output error criterion where an existing estimate of the parameters is iteratively improved until the model response is sufficiently close to that of the measured output. In a survey paper by *Kubrusly* [1977] on distributed parameter systems identification, the identification procedures have been classified into three categories: (1) direct method, which uses optimization techniques directly to the distributed (infinite dimensional) model; (2) reduction to a lumped parameter system, which reduces the distributed parameter system to a continuous or discrete-time lumped parameter system that is described by an ordinary differential equation or a difference equation; and (3) reduction to an algebraic equation, which reduces the partial differential equation to an algebraic equation.

There are two types of error criteria that have been used in the past in the formulation of the inverse problem for a distributed parameter system. *Chavent* [1979*b*] classified the identification procedures into two distinctive categories based upon the error criterion used in the formulations. His classification is intrinsically consistent with the work of *Neuman*[1973]. Hence, the inverse solution methods can be classified into the following two categories based upon the error criterion used in the formulation of the inverse problem.

Equation Error Criterion (Direct Method as Classified by Neuman)

If variations of states and the derivatives (usually estimated) of those state variables are known over the entire domain and if the measurement and model errors are negligible, the original governing equations become linear in terms of the unknown parameters. With the aid of boundary conditions, a direct solution for the unknown parameters may be possible.

In practice, only a limited number of observations of the state variables are available. To formulate the inverse problem by the equation error criterion, missing data (observations) have to be estimated by interpolation. The interpolated data in turn contain errors. If the interpolated data along with the observations, are substituted into the governing equations, some error terms will result. Such errors are called the equation errors. The errors are then minimized over the proper space of the parameters. It should be noted that approximating state variations in the entire domain using an interpolation scheme, without considering the statistical properties of sampling, would cause errors in the results of parameter identification.

Among the available techniques we may mention the energy dissipation method [*Nelson,* 1968]; linear programming [*Kleinecke,* 1971]; the use of a flatness criterion [*Emsellem and de Marsily,,* 1971]; the multiple objective decision process [*Neuman,* 1973]; the Galerkin method [*Frind and Pinder,* 1973]; the algebraic approach [*Sagar et al.,* 1975]; the inductive method [*Nutbrown,* 1975]; linear programming and quadratic programming [*Hefez,* 1975]; minimization of a quadratic objective function with penalty function [*Navarro,* 1977]; and the matrix inversion method [*Yeh et al.,* 1983]. To minimize the instability and nonuniqueness, regularity conditions are often required.

Output Error Criterion (Indirect Method as Classified by Neuman)

The criterion used in this approach is generally the minimization of a "norm" of the difference between observed and calculated states at specified observation points. The main advantage of this approach is that the formulation of the inverse problem is applicable to the situation where the number of observations is limited. It does not require differentiation of the measured data. Various optimization algorithms have been applied to perform the minimization. In general, an algorithm starts from a set of initial estimates of the parameters and improves it in an iterative manner until the system model response is sufficiently close to that of the observations.

Among the published works in parameter identification we may mention the following: quasilinearization [*Yeh and Tauxe,* 1971; *DiStefano and Rath,* 1973]; and maximum principle [*Lin and Yeh,* 1974], *Yakowitz and Noren* [1976]. *Vermuri and Karplus* [1969] formulated the inverse problem in terms of optimal control and solved it by a gradient procedure. *Chen et al.* [1974] and *Chavent* [1975] also treated the problem in an optimal control approach and solved it by both steepest descent method and the conjugate gradient method. Kalman filtering techniques have also been proposed in the literature for parameter identification [*McLaughlin,* 1975; *Wilson et al.,* 1978]. *Kitanidis and Vomvoris* [1983] used the technique of maximum likelihood estimation.

Mathematical programming techniques developed in the field of operations research have been utilized for solving the inverse problem of parameter identification in the field of petroleum engineering. Among the published works we may mention the following: gradient search procedures [*Jacquard and Jain,* 1965; *Thomas et al.,* 1972]; decomposition and multilevel optimization [*Haimes et al.,* 1968]; linear programming [*Coats et al.,* 1970; *Slater and Durrer,* 1971; *Yeh,* 1975*a, b*]; quadratic programming [*Yeh,* 1975*a, b; Chang and Yeh,* 1976]; the Gauss-Newton method [*Jahns,* 1966; *McLaughlin,* 1975]; the modified Gauss-Newton method [*Yoon and Yeh,* 1976; *Yeh and Yoon,* 1976; *Cooley,* 1977, 1982]; the Newton-Raphson method [*Neuman and Yakowitz,* 1979]; and the conjugate gradient method [*Neuman,* 1980].

1.2.3 Survey of Inverse Techniques

The heat conduction equation is given below to illustrate typical techniques that have been used to solve the inverse problem. Consider the following heat conduction equation:

$$\frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial T}{\partial y}\right)=C\frac{\partial T}{\partial t}+Q \tag{1.1}$$

subject to the initial and boundary conditions:

$$\begin{aligned} T(x,y,0) &= T_0(x,y) \quad x,y\in\Gamma=\Gamma_1+\Gamma_2 && (1.2)\\ T(x,y,t) &= T_1(x,y,t) \quad x,y\in\Gamma_1 && (1.3)\\ K\frac{\partial T}{\partial n} &= T_2(x,y,t) \quad x,y\in\Gamma_2 && (1.4)\end{aligned}$$

For illustrational purposes, let us assume that the source term, Q is known. The parameters chosen for identification are conductivity, K and heat capacity, C, which are assumed to be functions of x and t. In general, a numerical scheme is required to obtain solutions of (1.1) subject to conditions (1.2-1.4), provided that the values of the parameters, K and C, are properly prescribed. Various finite-difference or finite-element methods have been developed for numerical simulation. In solving the inverse problem, it is essential to have an efficient forward solution scheme. An example is Crank-Nicolson scheme:

$$\begin{aligned} & \frac{1}{2}\left[K^n_{i+\frac{1}{2},j}\left(\frac{T^{n+1}_{i+1,j}-T^{n+1}_{i,j}}{(\Delta x)^2}\right)-K^n_{i-\frac{1}{2},j}\left(\frac{T^{n+1}_{i,j}-T^{n+1}_{i-1,j}}{(\Delta x)^2}\right)\right]\\ + & \frac{1}{2}\left[K^n_{i+\frac{1}{2},j}\left(\frac{T^{n+1}_{i+1,j}-T^{n+1}_{i,j}}{(\Delta x)^2}\right)-K^n_{i-\frac{1}{2},j}\left(\frac{T^{n+1}_{i,j}-T^{n+1}_{i-1,j}}{(\Delta x)^2}\right)\right]\\ + & \frac{1}{2}\left[K^n_{i,j+\frac{1}{2}}\left(\frac{T^{n+1}_{i,j+1}-T^{n+1}_{i,j}}{(\Delta y)^2}\right)-K^n_{i,j-\frac{1}{2}}\left(\frac{T^{n+1}_{i,j}-T^{n+1}_{i,j-1}}{(\Delta y)^2}\right)\right]\\ + & \frac{1}{2}\left[K^n_{i,j+\frac{1}{2}}\left(\frac{T^{n+1}_{i,j+1}-T^{n+1}_{i,j}}{(\Delta y)^2}\right)-K^n_{i,j-\frac{1}{2}}\left(\frac{T^{n+1}_{i,j}-T^{n+1}_{i,j-1}}{(\Delta x)^2}\right)\right]\\ = & \; Q_{i,j}+C^n_{i,j}\left(\frac{T^{n+1}_{i,j}-T^{n+1}_{i,j}}{\Delta t}\right) \end{aligned} \tag{1.5}$$

The above finite-difference equations can be solvedfor $T^n_{i,j}$ by an alternating direction method [*Douglas*, 1962].

Generalized Matrix Method Based Upon the Equation Error Criterion

Suppose the temperature observations are available at each of the grid points and these observations are substituted into Equation (1.5); then the Crank-Nicolson scheme can be written as

$$
\begin{aligned}
& (T_{i+1,j}^{n+\frac{1}{2}} - T_{i,j}^{n+\frac{1}{2}})K_{i+1,j}^{n} - (T_{i,j}^{n+\frac{1}{2}} - T_{i-1,j}^{n+\frac{1}{2}})K_{i-1,j}^{n} \\
+ & (T_{i,j+1}^{n+\frac{1}{2}} - T_{i,j}^{n+\frac{1}{2}})K_{i,j+1}^{n} - (T_{i,j}^{n+\frac{1}{2}} - T_{i,j-1}^{n+\frac{1}{2}})K_{i,j-1}^{n} \\
+ & (T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} + T_{i,j+1}^{n+\frac{1}{2}} + T_{i,j-1}^{n+\frac{1}{2}} - 4T_{i,j}^{n+\frac{1}{2}})K_{i,j}^{n} \\
- & \frac{2(\Delta x)^2}{\Delta t}(T_{i,j}^{n+1} - T_{i,j}^{n})C_{i,j}^{n} \\
= & 2(\Delta x)^2 Q + \epsilon_{i,j}^{n+\frac{1}{2}}
\end{aligned}
\tag{1.6}
$$

where Δy is assumed to be equal to Δx, and

$$
\begin{aligned}
T_{i,j}^{n+\frac{1}{2}} &= \frac{1}{2}(T_{i,j}^{n+1} + T_{i,j}^{n}) \\
K_{i+\frac{1}{2},j}^{n} &= \frac{1}{2}(K_{i+1,j}^{n} + K_{i,j}^{n})
\end{aligned}
$$

To account for the lack of equality, an unknown error term $\epsilon_{i,j}^{n+\frac{1}{2}}$ is added to Equation (1.6). In practice, only a limited number of field observations is available. Interpolation schemes, such as cubic splines [*Yakowitz and Noren,* 1976] and kriging [*Yeh at al.,* 1983] have been applied in the past to obtain values of the state at every computational grid associated with the numerical scheme that is based upon either finite-difference or finite element approximations. The error term consists of interpolation errors as well as noise in observations. Equation (1.6) can be simplified to

$$A_i\ P_i = b_i + \epsilon_i \quad i = 1, 2, \cdots, N \tag{1.7}$$

with A_i the coefficient matrix, a function of T;
P_i the vector containing values of conductivity and heat capacity at all grid points;
N the total number of time steps; and
b_i the column vector, a function of T.
In more compact matrix form, this becomes

$$A\ P = b + \epsilon \quad i = 1, 2, \cdots, N \tag{1.8}$$

where

$$\begin{aligned} A &= [A_1^T, A_2^T, \cdots, A_N^T]^T \\ b &= [b_1^T, b_2^T, \cdots, b_N^T]^T \\ \epsilon &= [\epsilon_1^T, \epsilon_2^T, \cdots, \epsilon_N^T]^T \end{aligned}$$

and $[\ ]^T$ is a transpose operator. Whether the finite difference or the finite element is used as the forward solution method, the resulting equation error will always have the form of (1.8). However, a typical finite-difference method is used to demonstrate how to formulate the inverse problem by the equation error criterion. The vector of unknown parameters, P can be determined by minimizing the equation error ϵ.

From (1.8), the least squares error (or residual sum of squares) can be expressed by

$$\epsilon^T \epsilon = (A\ P - b)^T (A\ P - b) \tag{1.9}$$

Minimizing the least square error, the vector containing the parameters can be estimated as

$$\hat{P} = (A^T A)^{-1} A^T b \tag{1.10}$$

where $\hat{P}$ is the estimated vector of P. The solution is highly dependent on the level of discretization used in the numerical solution of the governing equation. Another disadvantage is that solution (1.10) is generally unstable in the presence of noise.

Gauss-Newton Minimization Based upon the Output Error Criterion

For modeling purposes, the objective is to determine $K(x, y, t)$ from a limited number of observations of $T(x, y, t)$ in the domain so that a certain cost function is optimized. If the classical least squares error is used to represent the output error, the objective function to be minimized is

$$\min_{K(x,y,t)} J = [A_T - A_Y]^T [A_T - A_Y] \tag{1.11}$$

where A_T is the vector of estimated temperatures based upon estimated values of parameter K, and A_Y is the vector of observed temperatures.

The Gauss-Newton algorithm has proven to be an effective algorithm to perform minimization. The original and modified version of the algorithm have been used by many researchers in the past in solving the inverse problem, e.g., *Jacquard and Jain* [1965]; *Jahns* [1966], *Thomas et al.* [1972], *Gavalas et al.* [1976], *Yoon and Yeh* [1976], and *Cooley* [1977,1982]. The popularity of the algorithm stems from the fact that it does not require the calculation of the Hessian matrix as is required by the Newton method and the rate of convergence is superior when compared to the classical gradient search procedures. The algorithm is basically developed from unconstrained minimization. However, constraints such as upper and lower bounds are easily incorporated in the algorithm with minor modifications. The algorithm starts with a set of initial estimates of parameters and converges to a local optimum. If the objective function is convex, the local optimum would be the global optimum. Due to the presence of noise in the observations, the inverse problem is usually nonconvex, and hence only a local optimum can be assured in the minimization.

Let $\bar{K}$ be a vector of parameters that contains $[K_1, K_2, \cdots, K_L]$. The algorithm generates the following parameter sequence for an unconstrained minimization problem:

$$\bar{K}^{n+1} = \bar{K}^n - \beta^n P^n \tag{1.12}$$

with

$$A^n P^n = g^n \tag{1.13}$$

where

$A^n = [J_K(\bar{K}^n)]^T [J_K(\bar{K}^n)], (L \times L)$;

$g^n = [J_K(\bar{K}^n)]^T [A_T - A_Y], (L \times 1)$;

J_K Jacobian matrix of temperature with respect to $\bar{K}$, $M \times L$;

β^n step size, (scalar);

P^n Gauss-Newton direction vector, $(L \times 1)$;

M number of observations;

L parameter dimension.

The elements of Jacobian matrix are represented by the sensitivity coefficients,

$$J_K = \begin{pmatrix} \frac{\partial T_1}{\partial K_1} & \frac{\partial T_1}{\partial K_1} & \cdots \frac{\partial T_1}{\partial K_L} \\ \frac{\partial T_2}{\partial K_1} & \frac{\partial T_2}{\partial K_2} & \cdots \frac{\partial T_2}{\partial K_L} \\ \cdots & \cdots & \cdots \\ \frac{\partial T_M}{\partial K_1} & \frac{\partial T_M}{\partial K_2} & \cdots \frac{\partial T_M}{\partial K_L} \end{pmatrix} \tag{1.14}$$

where M is the total number of observations, and L is the total number of parameters.

The step size β^n are determined by a quadratic interpolation scheme such that $J(K^{n+1}) < J(K^n)$, or simply by a trial-and-error procedure. Occasionally, the direction matrix $[J_K{}^T J_K]$ become ill-conditioned. As stated earlier, the original Gauss-Newton algorithm does not handle constraints.

In solving the inverse problem, we need to calculate the above sensitivity matrix in each iteration.

Conjugate Gradient Method

Neuman [1980] developed an efficient conjugate gradient algorithm for performing minimization of the objective function. He extended the variational method developed by *Chavent* [1975] for calculating the gradient of the functional with respect to the parameter. The conjugate gradient method uses a combination of negative gradient of the functional and previous descent direction as the latest search direction. In this case, the following iterative process is used for the estimation of K by minimizing the objective function (1.11)

$$\hat{K}^{n+1} = \hat{K}^n - \beta_K^n P_K^n \tag{1.15}$$

where β_K^n is step size for K in going from iteration n to iteration $n+1$, and P_K^n is direction of descent (i.e., search direction) for K. It is given by

$$P_K^n = J'^n_K + \nu_K^n P_K^{n-1} \tag{1.16}$$

which is the conjugation of (a) the gradient direction J'^n_K at iteration n and (b) the direction of descent P_K^{n-1} for K. The conjugate coefficient is given by

$$\nu_K^n = \frac{\int_{x=0}^{1} (J'^n_K)^2 dx}{\int_{x=0}^{1} (J'^{n-1}_K)^2 dx} \qquad \text{with} \quad \nu_K^0 = 0 \tag{1.17}$$

In this optimization method, the solution converges rapidly and is not as sensitive to the measurement errors as compared to Gauss-Newton or other conventional optimization technique. More recently, the method has been applied to the solution of the inverse heat conduction problem. *Huang and Ozisik* [1992] applied this optimization technique for determination of wall heat flux in laminar flow and contact conductance during metal casting. *Huang and Yan* [1995] employed this method for determination of conductivity and heat capacity.

1.3 Scope of the Present Work

The present study is concerned with the determination of parameters that arise in nonlinear diffusion-dominated problems. The parameters are not constant values; they depend intricately on the dependent variables themselves. They can be identified with physical properties such as thermal conductivity and heat capacity in heat conduction applications. They can also be interpreted as constitutive relationships required to model flow in an unsaturated porous medium.

The parameter estimation procedure adopted in the present work follows a broad-based 'inverse technique'. This technique is based on the minimization of a suitable cost function using a gradient search algorithm. This search is augmented by using the conjugate gradient method. Special features of the technique used are:

1. the use of the adjoint operator of the governing partial differential equation to construct the derivative of the cost function and
2. the use of sensitivity functions to identify clearly the portions of the measured data that seriously influence the predicted results.

Chapter 2

Mathematical Formulation

The mathematical procedure of the inverse method based on gradient search is explained for a variety of steady and unsteady problems in the present chapter. The original algorithm has been adapted from the work *C. H. Huang and Yan*(1995) and has been applied to steady and unsteady diffusion-like problems. The individual steps of the algorithm can be stated as follows:

1. Assume the property functions, namely the parameters to be estimated.
2. Solve the adjoint problem and obtain adjoint variables.
3. Compute the gradients of the objective function.
4. Compute the conjugate coefficients.
5. Compute the directions of descent.
6. Solve the sensitivity problems to obtain sensitivity functions.
7. Compute search step sizes.
8. Update the parameters to be estimated.
9. Repeat the above computational procedure until the convergence criterion is satisfied.

2.1 Definition of Direct and Inverse Problems

The governing equation of a physical problem can be symbolically represented as:

$$L(u, p; x, t) = 0 \tag{2.1}$$

where

$$u = (u_1, u_2 \cdots n_{nu})^T \tag{2.2}$$
$$p = (p_1, p_2 \cdots p_{np})^T \tag{2.3}$$
$$L = (L_1, L_2 \cdots L_{nu})^T \tag{2.4}$$

x is a spatial coordinate, t is time, $(u_1, u_2 \cdots u_{nu})$ are nu state variables and $(p_1, p_2 \cdots p_{np})$ are np parameters. The set $(L_1, L_2, \cdots, L_{nu})$ represents linear/nonlinear differential operators acting on the state variables $(u_1, u_2, \cdots, u_{nu})$. The initial and boundary conditions needed to solve Equation (2.1) are

$$u = f_0 \quad \text{when} \quad t = t_0 \tag{2.5}$$
$$L_{UB} = f_1 \quad \text{on} \quad \Gamma_{UB} \tag{2.6}$$
$$L_{LB} = f_2 \quad \text{on} \quad \Gamma_{LB} \tag{2.7}$$

L_{UB} and L_{LB} are vector operators representing boundary conditions on the surfaces Γ_{UB} and Γ_{LB} respectively.

2.1.1 Direct Problem

The direct problem is concerned with integrating the operator L, i.e. the estimation of the unknown state u when parameter p and all initial and boundary conditions are prescribed.

2.1.2 Inverse Problem

The inverse problem carries out the estimation of unknown parameters p or initial or boundary conditions when continuous or discrete observations of state u are given.

2.1.3 Sensitivity Analysis and Sampling

As discussed by *Knopman and Voss* [1987], the accuracy with which parameters can be estimated depends on the points in space and time at which the data for the inverse problem is collected. The parameter estimates will be accurate when the data for the inverse problem is obtained by sampling at points where the state variables have the highest sensitivity to the parameters. Examination of sensitivities is the starting point for designing the sampling experiment. Of interest is the magnitude of the sensitivity rather than its sign. Therefore the distribution in space and time, of the absolute sensitivities

$$S_i = \left| \frac{\partial u(x,t;p)}{\partial p_i} \right| \tag{2.8}$$

is investigated. Sensitivity coefficients S_i are to be computed for all the parameters p_i

2.2 Steady State Heat Conduction

2.2.1 Direct Problem

The following steady-state problem is first considered. A slab of thickness $\bar{L}$ is kept at two fixed temperatures at its two boundaries. The surface at $\bar{x} = 0$ is kept at a temperature $\bar{T}_l$ while the other boundary at $\bar{x} = \bar{L}$ is kept at $\bar{T}_r$. The governing equation for steady heat conduction in the slab is given by

$$\frac{d}{d\bar{x}}\left[\bar{K}(\bar{T})\frac{d\bar{T}}{d\bar{x}}\right] = 0 \tag{2.9}$$

$$\bar{T} = \bar{T}_0 \qquad \text{at} \quad \bar{x} = 0 \tag{2.10}$$

$$\bar{T} = \bar{T}_l \qquad \text{at} \quad \bar{x} = \bar{L} \tag{2.11}$$

With the following dimensionless quantities

$$x = \frac{\bar{x}}{\bar{L}}, \quad T = \frac{\bar{T}}{\bar{T}_r}, \quad K = \frac{\bar{T}}{\bar{T}_r}$$

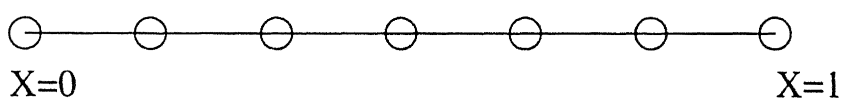

Figure 2.1: Thermocouple arrangement for measurements at M points

we get the following dimensionless form

$$\frac{d}{dx}\left[K(T)\frac{dT}{dx}\right] = 0 \qquad \text{in} \quad 0 < x < 1 \tag{2.12}$$

$$T = T_0 \qquad \text{for} \quad x = 0 \tag{2.13}$$

$$T = T_1 \qquad \text{for} \quad x = 1 \tag{2.14}$$

The direct problem is concerned with the determination of temperature in the slab when thermal conductivity and the boundary conditions at $x = 0$ and $x = 1$ are known.

2.2.2 Inverse Problem

For the inverse problem, thermal conductivity $K(T)$ is regarded as the unknown, but other quantities in Equations (2.12-2.14) are known. In addition, temperature readings taken at some appropriate locations are considered available. Referring to Figure 1, it is assumed that M sensors are used to record the temperature information to identify $K(T)$ in the inverse calculations. Let the temperature readings taken by these sensors be denoted by $Y_i(x_i) \equiv Y_i, i = 1, \cdots M$ where $i = 1$ and M always correspond to $x = 0$ and 1 (i.e. boundary measurements) respectively. Then the inverse problem can be stated as follows: by utilizing the measured temperature data, Y_i, estimate the unknown temperature-dependent thermal property, $K(T)$.

In the inverse calculations, the measured temperatures are known either from numerical simulation or from real experiments. Once the temperature field is known, there exist some unknown but fixed thermal property that its value (a number) $K(x)$, at any position, x, must satisfy the Fourier equation to give this known temperature distribution. Therefore, in the inverse problem of function estimation, one can replace $K(T)$ by $K(x)$. By using the minimization procedure of the objective function J, the function $K(x)$ (and then $K(T)$) can be determined. The inverse problem is generated by requiring that the following functional be minimized:

$$J[K(T)] \equiv J[K(x)] = \sum_{i=1}^{M}[T_i(\hat{k}) - Y_i(x_i)]^2 \tag{2.15}$$

Here, T_i are the estimated temperatures in the slab at the locations $x = x_i$. These quantities are determined from the solution of the direct problem (2.12-2.14) using an estimated $\hat{K}(x)$ for the exact $K(x)$. The measured temperatures at $x = x_i$ are denoted by Y_i.

2.2.3 Conjugate Gradient Method

The following iterative process based on the conjugate gradient method is now used for the estimation of $K(x)$ by minimizing the above functional $J[K(x)]$:

$$\hat{K}^{n+1}(x) = \hat{K}^{n}(x) - \beta_K^n P_K^n(x) \tag{2.16}$$

where β_K^n is the step size for K in going from the iteration number n to $n+1$ and P_K^n is the direction of descent (i.e. search direction) for K. It is given by

$$P_K^n(x) = J'^n_K(x) + \nu_K^n P_K^{n-1}(x) \tag{2.17}$$

This is the conjugation of the gradient direction J'^n_K at iteration n with respect to the direction of descent P_K^{n-1} at iteration number $n-1$. The conjugate coefficient is given by the recursion formula

$$\nu_K^n = \frac{\int_{x=0}^{1}(J'^n_K)^2 dx}{\int_{x=0}^{1}(J'^{n-1}_K)^2 dx} \qquad \text{with} \qquad \nu_K^0 = 0 \tag{2.18}$$

We note that when $\nu_K^n = 0$ for any n, in Equation (2.18), the direction of descent $P_K^n(x)$ becomes the gradient direction, i.e. the 'steepest-descent' method is obtained.

To perform the iterations according to Equation (2.16), we need to compute the step sizes β_K^n and the gradient of the functional J'^n_K. In order to develop expressions for the determination of these quantities, the 'sensitivity problem' and 'adjoint problem' are constructed as described below.

2.2.4 Sensitivity Analysis and Search Step Size

In order to derive the sensitivity problem, it is necessary to perturb K. It is assumed that when $K(x)$ undergoes a variation $\Delta K(x)$, $T(x)$ is perturbed by $T + \Delta T_K$. Then replacing k by $k + \Delta k$ and T by $T + \Delta T_K$ in the direct problem, subtracting from the resulting expressions and neglecting the second-order terms, the following problem for the sensitivity function ΔT_K is obtained

$$\frac{d}{dx}\left[K(x)\frac{d(\Delta T_K)}{dx}\right] + \frac{d}{dx}\left[\Delta K \frac{dT}{dx}\right] = 0 \tag{2.19}$$

$$\Delta T_K = 0 \qquad at \quad x = 0 \tag{2.20}$$

$$\Delta T_K = 0 \qquad at \quad x = 1 \tag{2.21}$$

This system can be solved as a direct problem for ΔT_K. The functional (2.15) for iteration $n+1$ then becomes

$$\begin{aligned} J(\hat{k}^{n+1}) &= \sum_{i=1}^{m}[T_i(\hat{k}^n - \beta_k^n P_k^n) - Y_i]^2 \\ &= \sum_{i=1}^{m}[T_i(\hat{k}^n) - \beta_k^n (P_k^n \tfrac{dT}{dk})_i - Y_i]^2 \\ &= \sum_{i=1}^{m}[T_i(\hat{k}^n) - \beta_k^n (\Delta T_k^n)_i - Y_i]^2 \end{aligned} \tag{2.22}$$

In this derivation, it is assumed that $\Delta K = P_K^n$ and $\Delta T_K^n(x_i) = (P_k^n \frac{dT}{dk})_i$
The step sizes β_k^n are calculated in such a way that $J(\hat{k}^{n+1})$ is a minimum. Thus

$$\frac{\partial J(\hat{K}^{n+1})}{\partial \beta_K^n} = 0$$

leading to

$$\beta_K^n = \frac{\sum_{i=1}^{m}(T_i^n - Y_i)(\Delta T_K^n)_i}{\sum_{i=1}^{m}[(\Delta T_K^n)_i]^2} \tag{2.23}$$

The sensitivity function ΔT_K^n required in this formula is calculated from Equations 2.19-2.21. To apply Equation 2.16, the gradient of the objective function J is needed. This is calculated as follows:

2.2.5 Adjoint Problem and Gradient Equation

To derive the adjoint problem for $K(x)$, Equation (2.12) is multiplied by the adjoint function $\lambda(x)$ and the resulting expression is integrated over the space domain. Then the result is added to the right-hand side of equation (2.15) to yield the following expression for the functional $J[K(x)]$:

$$J[K(x)] = \int_{x=0}^{1} \lambda \left[\frac{d}{dx}\left(K(T)\frac{dT(x)}{dx}\right)\right] dx + \sum_{i=1}^{M}(T_i - Y_i)^2 \tag{2.24}$$

The functional $J[K(T)]$ is discrete due to the last term of Equation (2.24). To make this functional continuous we introduce the Dirac delta function. Then the functional can be written as

$$J[K(x)] = \int_{x=0}^{1} \lambda \left[\frac{d}{dx}\left(K(T)\frac{dT(x)}{dx}\right)\right] dx + \int_{x=0}^{1} \sum_{i=1}^{m}[T - Y]^2 \delta(x - x_i) dx \tag{2.25}$$

which is continuous in the sense of theory of distributions.

The variation of the functional ΔJ_K due to variation of K, is obtained by perturbing T by $T + \Delta T_K$ and K by $K + \Delta K$ in Equation (2.25), subtracting from the resulting expression the original Equation (2.25) and neglecting the higher-order terms. We thus obtain

$$\Delta J_K = \int\limits_{x=0}^{1} \lambda \left[\frac{d}{dx}\left(K(x)\frac{d(\Delta T_K)}{dx}\right) + \frac{d}{dx}\left(\Delta K\frac{dT}{dx}\right)\right] dx$$

$$+2\int_{x=0}^{1}\sum_{i=1}^{m}[T-Y]\Delta T_K \delta(x-x_i)dx \qquad (2.26)$$

$$\text{Or}\quad \Delta J_K = \left[\lambda K(x)\frac{d(\Delta T_K)}{dx}\right]_{x=0}^{1} - \int\limits_{x=0}^{1} K(x)\frac{d\lambda}{dx}\left[\frac{d(\Delta T_K)}{dx}\right] dx$$

$$+\left[\lambda\Delta K\frac{dT}{dx}\right]_{x=0}^{1} - \int\limits_{x=0}^{1}\Delta K\left[\frac{d\lambda}{dx}\frac{dT}{dx}\right] dx + 2[(T-Y)\Delta T_K]_{x=1}$$

$$+2[(T-Y)\Delta T_K]_{x=0} + 2\int_{x=0}^{1}\sum_{i=2}^{M-1}[T-Y]\Delta T_K\delta(x-x_i)dx$$

$$\text{Or}\quad \Delta J_K = \left[\lambda K(x)\frac{d(\Delta T_K)}{dx}\right]_{x=0}^{1} - \left[\Delta T_K K(x)\frac{d\lambda}{dx}\right]_{x=0}^{1} + \int\limits_{x=0}^{1}\Delta T_K\left[\frac{d}{dx}\left(K(x)\frac{d\lambda}{dx}\right)\right] dx$$

$$+\left[\lambda\Delta K\frac{dT}{dx}\right]_{x=0}^{1} - \int\limits_{x=0}^{1}\Delta K\left[\frac{d\lambda}{dx}\frac{dT}{dx}\right] dx + 2[(T-Y)\Delta T_K]_{x=1}$$

$$+2[(T-Y)\Delta T_K]_{x=0} + 2\int_{x=0}^{1}\sum_{i=2}^{M-1}[T-Y]\Delta T_K\delta(x-x_i)dx \qquad (2.27)$$

From sensitivity Equation (2.19)we see that ΔT_K vanishes at the two boundaries. Hence Equation (2.27) reduces to

$$\Delta J_K = \left[\lambda K(x)\frac{d(\Delta T_K)}{dx}\right]_{x=0}^{1} + \int\limits_{x=0}^{1}\Delta T_K\left[\frac{d}{dx}\left(K(x)\frac{d\lambda}{dx}\right) + \sum_{i=2}^{M-1}[T-Y]\delta(x-x_i)\right] dx$$

$$+\left[\lambda\Delta K\frac{dT}{dx}\right]_{x=0}^{1} - \int_{x=0}^{1} \Delta K\left[\frac{d\lambda}{dx}\frac{dT}{dx}\right]dx \tag{2.28}$$

Since ΔJ_K depends only on ΔK but does not depend on $(\Delta T)_K$, the integrands containing ΔT_K should be zero. Hence we have

$$\frac{d}{dx}\left(K(x)\frac{d\lambda}{dx}\right) + \sum_{i=2}^{M-1}[T-Y]\delta(x-x_i) = 0 \tag{2.29}$$

$$\lambda = 0 \quad \text{at} \quad x = 0 \quad \text{and} \quad x = 1 \tag{2.30}$$

Equation (2.28) thus reduces to

$$\Delta J_K = -\int_{x=0}^{1} \Delta K(x)\left[\frac{d\lambda}{dx}\frac{dT}{dx}\right]dx \tag{2.31}$$

From the definition of ΔJ_K we have

$$\Delta J_K = \int_{x=0}^{1} J'_K(x)\Delta K(x)dx \tag{2.32}$$

Comparing Equations (2.31) and (2.32) we get the following expression for the gradient $J'_K(x)$ of the functional J:

$$J'_K(x) = -\frac{d\lambda}{dx}\frac{dT}{dx} \tag{2.33}$$

where T is calculated from direct problem (2.12-2.14) and λ from the adjoint Equation (2.29-2.30).

2.2.6 Discrepancy Principle for Stopping Criteria

If the problem involves no measurement errors, the traditional convergence check specified as

$$|J| < \epsilon \tag{2.34}$$

where ϵ is a small specified number, can be used as the stopping criterion. However, the observed temperature information contains measurement errors; as a result, the inverse solution will tend to approach the perturbed input data, and the solution will exhibit

oscillatory behavior as the number of iterations is increased. Computational experience has shown that it is useful to use the discrepancy principle for terminating the iteration process in the regular method. Assuming $T(x_i) - Y(x_i) \cong \sigma$, the discrepancy principle that establishes the value of the stopping criterion ϵ can be obtained from Equation (2.15) as

$$\int_0^1 \sigma^2 \, dx \equiv \epsilon^2 \tag{2.35}$$

where σ is the standard deviation of the measurement error. Then the stopping criterion is taken as

$$|J| < \epsilon^2 \tag{2.36}$$

where ϵ is determined from Equation (2.35). In the present analysis the following stopping criterion is used

$$|J^{n+1} - J^n| \leq \epsilon \tag{2.37}$$

The iterative procedure for calculating the function $K(x)$ can be summarized as follows:

1. Assume the form of $K(x)$; a constant function is a useful starting point.
2. Generate the corresponding temperature field $T(x)$, by solving Equations (2.12-2.14).
3. Solve the adjoint problem, Equations (2.29-2.30), and obtain adjoint variable $\lambda(x)$.
4. Compute J'_K from Equation (2.33).
5. Calculate the conjugate coefficient ν_K using Equation (2.18).
6. Estimate the direction of descent P_K, from Equation (2.17).
7. Solve the sensitivity problem, Equations (2.19- 2.21), and obtain ΔT_K.
8. Compute step size β_K using Equation (2.23).
9. Estimate K using Equation (2.16).
10. Repeat the above calculation procedure until the discrepancy principle is satisfied.

At convergence, $J \to 0$, $T(x_i)$ will be close to the measured data Y_i and so the property $K(T)$ can be recovered by correlating $K(x)$ and $T(x)$.

2.3 Transient Heat Conduction

The procedure presented above for steady heat conduction is now extended to include transient heat conduction.

2.3.1 Flux-Flux Boundary Conditions

Direct Problem

We consider the following unsteady heat conduction problem. A slab of thickness $\bar{L}$ is initially at temperature $\bar{T}_0$. The boundary at $\bar{x} = 0$ is subjected to a constant heat flux $\bar{q}_l$ while the other boundary at $\bar{x} = \bar{L}$ is insulated. The governing differential equation of the physical problem can be written as

$$\frac{\partial}{\partial \bar{x}}\left(\bar{K}(\bar{T})\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}}\right) = \bar{\rho}\bar{C}(\bar{T})\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{t}} \qquad \text{in } 0 < \bar{x} < \bar{L} \tag{2.38}$$

$$-\bar{K}(\bar{T})\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} = \bar{q}_l \qquad \text{at } \bar{x} = 0 \tag{2.39}$$

$$-\bar{K}(\bar{T})\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} = \bar{q}_r \qquad \text{at } \bar{x} = \bar{L} \tag{2.40}$$

$$T(x,t) = T_0 \qquad \text{for } t = 0 \tag{2.41}$$

With the following dimensionless variables

$$x = \frac{\bar{x}}{\bar{L}}, \quad T = \frac{\bar{T}}{\bar{T}_r}, \quad T_0 = \frac{\bar{T}_0}{\bar{T}_r}, \quad K = \frac{\bar{K}}{\bar{K}_r}$$

$$t = \frac{\bar{K}_r\bar{t}}{\bar{\rho}\bar{C}_r\bar{L}^2}, \quad q_l = \frac{\bar{L}\bar{q}_l}{\bar{K}_r\bar{T}_r}, \quad q_r = \frac{\bar{L}\bar{q}_r}{\bar{K}_r\bar{T}_r}, \quad C = \frac{\bar{C}}{\bar{C}_r}$$

we obtain dimensionless form of Equations (2.38 -2.41) as follows:

$$\frac{\partial}{\partial x}\left(K(T)\frac{\partial T(x,t)}{\partial x}\right) = C(T)\frac{\partial T(x,t)}{\partial t} \qquad \text{in } 0 < x < 1 \tag{2.42}$$

$$-K(T)\frac{\partial T(x,t)}{\partial x} = q_l \qquad \text{at } x = 0 \tag{2.43}$$

$$-K(T)\frac{\partial T(x,t)}{\partial x} = q_r \qquad \text{at } x = 1 \tag{2.44}$$

$$T(x,t) = T_0 \qquad \text{for } t = 0 \tag{2.45}$$

The overbar '-' and the subscript 'r' denote dimensional and reference quantities, respectively.

There are two unknown parameters, $K(T)$ and $C(T)$ to be determined from a single differential equation. Hence there is a need to calculate sensitivity functions, adjoint functions and gradient equations for both K and C.

Sensitivity Problem and Step Size

The sensitivity function ΔT_K is defined as the change in estimated temperatures at different positions and times due to a change ΔK in $K(x,t)$. From (2.42-2.45) we get the equations governing the sensitivity function ΔT_K as follows:

$$\begin{aligned} \frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \Delta T_K(x,t)}{\partial x}\right) &+ \frac{\partial}{\partial x}\left(\Delta K(x,t)\frac{\partial T(x,t)}{\partial x}\right) \\ &= C\frac{\partial \Delta T_K(x,t)}{\partial x} \quad \text{for } 0<x<1 \qquad (2.46) \\ -K(x,t)\frac{\partial \Delta T_K(x,t)}{\partial x} &= \Delta K(x,t)\frac{\partial T(x,t)}{\partial x} \quad \text{for } x=0 \qquad (2.47) \\ -K(x,t)\frac{\partial \Delta T_K(x,t)}{\partial x} &= \Delta K(x,t)\frac{\partial T(x,t)}{\partial x} \quad \text{for } x=1 \qquad (2.48) \\ \Delta T_K(x,t) &= 0 \quad \text{for } t=0 \qquad (2.49) \end{aligned}$$

Similarly, the sensitivity function ΔT_C corresponding to the property C is given by

$$\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \Delta T_C(x,t)}{\partial x}\right) = C\frac{\partial \Delta T_C(x,t)}{\partial x} + \Delta C(x,t)\frac{\partial T(x,t)}{\partial x} \quad \text{for } 0<x<1 \qquad (2.50)$$

$$\frac{\partial \Delta T_C(x,t)}{\partial x} = 0 \quad \text{for } x=0 \qquad (2.51)$$

$$\frac{\partial \Delta T_C(x,t)}{\partial x} = 0 \quad \text{for } x=1 \qquad (2.52)$$

$$\Delta T_C(x,t) = 0 \quad \text{for } t=0 \qquad (2.53)$$

The solution of the inverse problem i.e.$K(x,t)$ and$C(x,t)$ is to be obtained in such a way that the difference between estimated results and experimental results is minimized. Here we want to minimize the sum of squares of differences between the estimated results and

experimental results at different points of the slab over a time period t_f. Therefore, the objective functional can be written as

$$J[K(T), C(T)] = \int_{t=0}^{t_f} \sum_{i=1}^{m} [T_i(\hat{K}, \hat{C}) - Y_i(x_i, t)]^2 dt \tag{2.54}$$

where, $Y_i(x_i, t)$ is the temperature reading taken with a sensor placed at $x = x_i$ at time t. M sensors are used to record temperature history over a time t_f. All the sensors are assumed be uniformly placed.

The following iterative process based on the conjugate gradient method is now proposed to update the properties:

$$\hat{K}^{n+1}(x,t) = \hat{K}^n(x,t) - \beta_K^n P_K^n(x,t) \tag{2.55}$$

$$\hat{C}^{n+1}(x,t) = \hat{C}^n(x,t) - \beta_C^n P_C^n(x,t) \tag{2.56}$$

The directions of descent for K and C are as follows

$$P_K^n(x,t) = J'^n_K(x,t) + \nu_K^n P_K^{n-1}(x,t) \tag{2.57}$$

$$P_C^n(x,t) = J'^n_C(x,t) + \nu_C^n P_C^{n-1}(x,t) \tag{2.58}$$

The sensitivity coefficients for K and C are given by

$$\nu_K^n = \frac{\int_{t=0}^{t_f} \int_{x=0}^{1} (J'^n_K)^2 dx dt}{\int_{t=0}^{t_f} \int_{x=0}^{1} (J'^{n-1}_K)^2 dx dt} \tag{2.59}$$

$$\nu_C^n = \frac{\int_{t=0}^{t_f} \int_{x=0}^{1} (J'^n_C)^2 dx dt}{\int_{t=0}^{t_f} \int_{x=0}^{1} (J'^{n-1}_C)^2 dx dt} \tag{2.60}$$

The functional $J(\hat{K}^{n+1}, \hat{C}^{n+1})$ for iteration $n+1$ is obtained as follows

$$J(\hat{K}^{n+1}, \hat{C}^{n+1}) = \int_{t=0}^{t_f} \sum_{i=1}^{M} [T_i(\hat{K}^n - \beta_K^n P_K^n,\ \hat{C}^n - \beta_C^n P_C^n) - Y_i]^2\ dt \tag{2.61}$$

Expanding the above expression of the functional using Taylor series and neglecting higher-order terms we have

$$J(\hat{K}^{n+1}, \hat{C}^{n+1}) = \int_{t=0}^{t_f} \sum_{i=1}^{M} [T_i(\hat{K}^n, \hat{C}^n) - \beta_K^n (\Delta T_K^n)_i - \beta_C^n (\Delta T_C^n)_i - Y_i]^2 dt \tag{2.62}$$

here the following assumptions are made.

$$\Delta T_K^n = P_K^n \frac{\partial T^n}{\partial K}$$
$$\Delta T_C^n = P_C^n \frac{\partial T^n}{\partial C}$$

The step sizes β_K^n and β_C^n are to be estimated in such a way that the objective function is minimized at $n+1$ iteration. Thus we have

$$\frac{J(\hat{K}^{n+1}, \hat{C}^{n+1})}{\partial \beta_K^n} = 0 \tag{2.63}$$
$$\frac{J(\hat{K}^{n+1}, \hat{C}^{n+1})}{\partial \beta_C^n} = 0 \tag{2.64}$$

which produce the following two linear equations for β_K^n and β_C^n.

$$a_{11}\beta_K^n + a_{12}\beta_C^n = b_1 \tag{2.65}$$
$$a_{21}\beta_K^n + a_{22}\beta_C^n = b_2 \tag{2.66}$$

where

$$a_{11} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_K^n)]_i^2 dt \tag{2.67}$$
$$a_{12} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_K^n)(\Delta T_C^n)]_i dt \tag{2.68}$$
$$a_{22} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_C^n)]_i^2 dt \tag{2.69}$$
$$a_{21} = a_{12} \tag{2.70}$$
$$b_1 = \int_{t=0}^{t_f} \sum_{i=1}^{M} (T_i^n - Y_i)(\Delta T_K^n)_i \; dt \tag{2.71}$$
$$b_2 = \int_{t=0}^{t_f} \sum_{i=1}^{M} (T_i^n - Y_i)(\Delta T_C{}^n)_i \; dt \tag{2.72}$$

From Equations (2.65-2.65) we get the following simplified expressions of step sizes β_K^n and β_C^n.

$$\beta_K^n = \frac{(b_1 a_{22} - b_2 a_{12})}{(a_{11}a_{22} - a_{12}^2)} \tag{2.73}$$
$$\beta_C^n = \frac{(b_2 a_{11} - b_1 a_{12})}{(a_{11}a_{22} - a_{12}^2)} \tag{2.74}$$

The gradient of the objective function is calculated using the adjoint problem approach as follows.

Adjoint Problem and Gradient Equation

To derive the adjoint problem for $K(x,t)$, Equation (2.42) is multiplied by the Lagrange multiplier $\lambda(x,t)$ and the resulting expression is integrated over the time and space domains. Then the result is added to the right-hand side of Equation (2.54). Hence the resulting expression of the functional $J[K(x,t), C(x,t)]$ becomes

$$J[K(x,t), C(x,t)] = \int_{t=0}^{t_f} \int_{x=0}^{1} \lambda \left[\frac{\partial}{\partial x} \left(K(T) \frac{\partial T(x,t)}{\partial x} \right) - C(T) \frac{\partial T(x,t)}{\partial t} \right] dx dt$$

$$+ \int_{t=0}^{t_f} \sum_{i=1}^{m} [T_i(x_i,t) - Y_i(x_i,t)]^2 dt \tag{2.75}$$

The variation ΔJ_K is obtained by perturbing T by ΔT_K in Equation (2.75), subtracting from the resulting expression the original Equation (2.75) and neglecting the higher-order terms. We thus obtain

$$\Delta J_K = \int_{t=0}^{t_f} \int_{x=0}^{1} \lambda \left[\frac{\partial}{\partial x} \left(K(x,t) \frac{\partial (\Delta T_K)}{\partial x} \right) + \frac{\partial}{\partial x} \left(\Delta K \frac{\partial T}{\partial x} \right) - C \frac{\partial \Delta T_K}{\partial t} \right] dx dt$$

$$+2 \int_{t=0}^{t_f} \int_{x=0}^{1} \sum_{i=1}^{m} [T - Y] \Delta T_K \delta(x - x_i) dx dt \tag{2.76}$$

Or $\Delta J_K =$

$$\int_{t=0}^{t_f} \left[\lambda K(x,t) \frac{\partial (\Delta T_K)}{\partial x} \right]_{x=0}^{1} dt - \int_{t=0}^{t_f} \int_{x=0}^{1} K(x,t) \frac{\partial \lambda}{\partial x} \left[\frac{\partial (\Delta T_K)}{\partial x} \right] dx dt$$

$$+ \int_{t=0}^{t_f} \left[\lambda \Delta K \frac{\partial T}{\partial x} \right]_{x=0}^{1} dt - \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta K \left[\frac{\partial \lambda}{\partial x} \frac{\partial T}{\partial x} \right] dx dt$$

$$- \int_{x=0}^{1} [C \lambda \Delta T_K]_{t=0}^{t_f} dx + \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta T_K \frac{\partial (C\lambda)}{\partial t} dx dt$$

$$+ \quad 2\int_{t=0}^{t_f} [(T-Y)\Delta T_K]_{x=1} dt + 2\int_{t=0}^{t_f} [(T-Y)\Delta T_K]_{x=0} dt$$

$$+ \quad 2\int_{t=0}^{t_f}\int_{x=0}^{1} \sum_{i=2}^{M-1} [T-Y]\Delta T_K \delta(x-x_i) dx dt$$

Or $\Delta J_K =$

$$\int_{t=0}^{1} \left[\lambda K(x,t)\frac{\partial(\Delta T_K)}{\partial x}\right]_{x=0}^{1} dt + \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta T_K \left[\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \lambda}{\partial x}\right)\right] dx dt$$

$$- \int_{t=0}^{t_f} \left[\Delta T_K K(x,t)\frac{\partial \lambda}{\partial x}\right]_{x=0}^{1} dt + \int_{t=0}^{t_f} \left[\lambda \Delta K \frac{\partial T}{\partial x}\right]_{x=0}^{1} dt - \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta K \left[\frac{\partial \lambda}{\partial x}\frac{\partial T}{\partial x}\right] dx dt$$

$$- \int_{x=0}^{1} [C\lambda \Delta T_K]_{t=0}^{t_f} dx + \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta T_K \frac{\partial (C\lambda)}{\partial t} dx dt + 2\int_{t=0}^{t_f} [(T-Y)\Delta T_K]_{x=1} dt$$

$$+ \quad 2\int_{t=0}^{t_f} [(T-Y)\Delta T_K]_{x=0} dt + 2\int_{t=0}^{t_f}\int_{x=0}^{1} \sum_{i=2}^{M-1} [T-Y]\Delta T_K \delta(x-x_i) dx dt$$

Or $\Delta J_K =$

$$\int_{t=0}^{t_f}\int_{x=0}^{1} \Delta T_K \left[\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \lambda}{\partial x}\right) + \frac{\partial (C\lambda)}{\partial t} + 2\sum_{i=2}^{M-1} [T-Y]\delta(x-x_i)\right] dx dt$$

$$+ \int_{t=0}^{t_f} \Delta T_K \left[K(x,t)\frac{\partial \lambda}{\partial x} + 2(T-Y)\right]_{x=0} dt$$

$$- \int_{t=0}^{t_f} \Delta T_K \left[K(x,t)\frac{\partial \lambda}{\partial x} - 2(T-Y)\right]_{x=1} dt$$

$$- \int_{x=0}^{1} [C\lambda \Delta T_K]_{t=0}^{t_f} dx + \int_{t=0}^{1} \lambda \left[K(x,t)\frac{\partial (\Delta T_K)}{\partial x} + \Delta K \frac{\partial T}{\partial x}\right]_{x=0}^{1} dt$$

$$- \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta K \left[\frac{\partial \lambda}{\partial x}\frac{\partial T}{\partial x}\right] dx dt \tag{2.77}$$

From the sensitivity problem at the two boundaries we get

$$K(x,t)\frac{\partial (\Delta T_K)}{\partial x} + \Delta K \frac{\partial T}{\partial x} = 0 \tag{2.78}$$

Note that ΔJ_K is not a function ΔT_K. Therefore the integrands containing ΔT_K should be zero. We thus get

$$\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \lambda}{\partial x}\right)+\frac{\partial (C\lambda)}{\partial t}+2\sum_{i=2}^{M-1}[T-Y]\delta(x-x_i)=0 \tag{2.79}$$

$$K(x,t)\frac{\partial \lambda}{\partial x}+2(T-Y)=0 \qquad \text{at} \quad x=0 \tag{2.80}$$

$$K(x,t)\frac{\partial \lambda}{\partial x}-2(T-Y)=0 \qquad \text{at} \quad x=1 \tag{2.81}$$

$$\lambda=0 \qquad \text{at} \quad t=t_f \tag{2.82}$$

Equation (2.77) reduces to

$$\Delta J_K=-\int\limits_{t=0}^{t_f}\int\limits_{x=0}^{1}\Delta K\left[\frac{\partial \lambda}{\partial x}\frac{\partial T}{\partial x}\right]dxdt \tag{2.83}$$

The expression for the variation of the functional ΔJ_C due to C is derived next. Following the same procedure as for property K we get

$$\begin{aligned}\Delta J_C &= \int\limits_{t=0}^{t_f}\int\limits_{x=0}^{1}\lambda\left[\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial(\Delta T_C)}{\partial x}\right)-\left(\Delta C\frac{\partial T}{\partial t}\right)-C\frac{\partial \Delta T_C}{\partial t}\right]dxdt\\ &+ 2\int\limits_{t=0}^{t_f}\int\limits_{x=0}^{1}\sum_{i=1}^{m}[T-Y]\Delta T_C\delta(x-x_i)dxdt\end{aligned} \tag{2.84}$$

Or $\Delta J_C =$

$$\begin{aligned}&\int\limits_{t=0}^{t_f}\left[\lambda K(x,t)\frac{\partial(\Delta T_C)}{\partial x}\right]_{x=0}^{1}dt-\int\limits_{t=0}^{t_f}\int\limits_{x=0}^{1}K(x,t)\frac{\partial \lambda}{\partial x}\left[\frac{\partial(\Delta T_C)}{\partial x}\right]dxdt\\ -&\int\limits_{t=0}^{t_f}\int\limits_{x=0}^{1}\Delta C\left[\lambda\frac{\partial T}{\partial t}\right]dxdt-\int\limits_{x=0}^{1}[C\lambda\Delta T_C]_{t=0}^{t_f}dx\\ +&\int\limits_{t=0}^{t_f}\int\limits_{x=0}^{1}\left[\frac{\partial(C\lambda)}{\partial t}\right]\Delta T_C dxdt+2\int\limits_{t=0}^{t_f}[(T-Y)\Delta T_C]_{x=1}dt\\ +&2\int\limits_{t=0}^{t_f}[(T-Y)\Delta T_C]_{x=0}dt+2\int\limits_{t=0}^{t_f}\int\limits_{x=0}^{1}\sum_{i=2}^{M-1}[T-Y]\Delta T_C\delta(x-x_i)dxdt\end{aligned}$$

Or $\Delta J_C =$

$$
\begin{aligned}
&\int_{t=0}^{t_f}\left[\lambda K(x,t)\frac{\partial(\Delta T_C)}{\partial x}\right]_{x=0}^{1} - \int_{t=0}^{t_f}\left[\Delta T_C K(x,t)\frac{\partial\lambda}{\partial x}\right]_{x=0}^{1} dt \\
+ &\int_{t=0}^{t_f}\int_{x=0}^{1} \Delta T_C\left[\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial\lambda}{\partial x}\right)\right] dxdt \\
- &\int_{t=0}^{t_f}\int_{x=0}^{1} \Delta C\left[\lambda\frac{\partial T}{\partial t}\right] dxdt - \int_{x=0}^{1}[C\lambda\Delta T_C]_{t=0}^{t_f}dx \\
+ &\int_{t=0}^{t_f}\int_{x=0}^{1}\left[\frac{\partial(C\lambda)}{\partial t}\right]\Delta T_C dxdt + 2\int_{t=0}^{t_f}[(T-Y)\Delta T_C]_{x=1}dt \\
+ &\ 2\int_{t=0}^{t_f}[(T-Y)\Delta T_C]_{x=0}dt \\
+ &\ 2\int_{t=0}^{t_f}\int_{x=0}^{1}\sum_{i=2}^{M-1}[T-Y]\Delta T_C\delta(x-x_i)dxdt
\end{aligned}
\tag{2.85}
$$

From the sensitivity equation (2.51-2.52) we have

$$
K(x)\frac{\partial(\Delta T_C)}{\partial x} = 0 \qquad \text{at} \quad x=0 \qquad \text{and} \quad x=1
$$

Hence the first integrand of Equation (2.85) will vanish. Thus we have

$$
\begin{aligned}
\Delta J_C = &\int_{t=0}^{t_f}\int_{x=0}^{1}\Delta T_C\left[\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial\lambda}{\partial x}\right) + \frac{\partial(C\lambda)}{\partial t} + 2\sum_{i=2}^{M-1}[T-Y]\delta(x-x_i)\right] dxdt \\
+ &\int_{t=0}^{t_f}\Delta T_C\left[K(x,t)\frac{\partial\lambda}{\partial x} + 2(T-Y)\right]_{x=0} dt \\
- &\int_{t=0}^{t_f}\Delta T_C\left[K(x,t)\frac{\partial\lambda}{\partial x} - 2(T-Y)\right]_{x=1} dt \\
- &\int_{x=0}^{1}[C\lambda\Delta T_C]_{t=0}^{t_f}dx - \int_{t=0}^{t_f}\int_{x=0}^{1}\Delta C\left[\lambda\frac{\partial T}{\partial x}\right] dxdt
\end{aligned}
\tag{2.86}
$$

Note that ΔJ_C should not depend on ΔT_C. Therefore the integrands containing ΔT_C are zero. Thus we have

$$
\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial\lambda}{\partial x}\right) + \frac{\partial(C\lambda)}{\partial t} + 2\sum_{i=2}^{M-1}[T-Y]\delta(x-x_i) = 0 \tag{2.87}
$$

$$K(x,t)\frac{\partial\lambda}{\partial x} + 2(T - Y) = 0 \qquad \text{for} \quad x = 0 \tag{2.88}$$

$$K(x,t)\frac{\partial\lambda}{\partial x} - 2(T - Y) = 0 \qquad \text{for} \quad x = 1 \tag{2.89}$$

$$\lambda = 0 \qquad \text{for} \quad t = t_f \tag{2.90}$$

From the sensitivity equation (2.53) we see that ΔT_C is zero at $t = 0$. Equation (2.86) is thus reduced to

$$\Delta J_C = -\int_{t=0}^{t_f}\int_{x=0}^{1}\left[\lambda\frac{\partial T}{\partial t}\right]\Delta C dx dt \tag{2.91}$$

Comparing the Equations (2.79-2.82) and (2.87-2.90) we see that the adjoint equations for K and C are similar.

The perturbations ΔJ_K and ΔJ_C can be defined as

$$\Delta J_K = \int_{t=0}^{t_f}\int_{x=0}^{1} J'_K(x,t)\Delta K dx dt \tag{2.92}$$

$$\Delta J_C = \int_{t=0}^{t_f}\int_{x=0}^{1} J'_C(x,t)\Delta C dx dt \tag{2.93}$$

Comparing (2.83) and (2.92) we get the following expression for the gradient of the functional with respect to K:

$$J'_K(x,t) = -\frac{\partial\lambda}{\partial x}\frac{\partial T}{\partial x} \tag{2.94}$$

Comparing equations (2.91) and (2.93) we get the gradient of the functional with respect to C:

$$J'_C(x,t) = -\lambda(x,t)\frac{\partial T(x,t)}{\partial x} \tag{2.95}$$

The gradient search procedure for obtaining the property functions K and C can be constructed as follows:

1. Assume the properties $K(x,t)$ and $C(x,t)$; In the absence of additional information, they can be treated as constants.

2. Generate the corresponding temperature field $T(x,t)$, by solving Equations (2.42-2.45).

3. Solve the adjoint problem, Equations (2.79-2.82), and obtain adjoint variable $\lambda(x,t)$.

4. Compute J'_K and J'_C from Equations (2.94) and (2.95)

5. Calculate the conjugate coefficients ν_K and ν_C using Equations (2.59) and (2.60) respectively.

6. Estimate the directions of descent P_K and P_C from Equations (2.57) and (2.58) respectively.

7. Solve the sensitivity problem, Equations (2.46- 2.49) and (2.50-2.53) to obtain sensitivity functions, ΔT_K and ΔT_C.

8. Compute step sizes β_K and β_C using Equations (2.73-2.74).

9. Estimate K and C using Equations (2.55-2.56).

10. Repeat the above calculation procedure until the discrepancy principle given by Equation (2.36) is satisfied.

2.3.2 Flux-Temperature Boundary Conditions

Direct Problem

Consider the following transient inverse heat conduction problem. A slab of thickness $\bar{L}$ is initially at temperature $\bar{T}_0$. The boundary surface at $\bar{x}=0$ is subjected to constant heat flux $\bar{q}_l$ while the other boundary at $\bar{x}=\bar{L}$ is insulated. Then the GDE of the physical problem can be written as

$$\frac{\partial}{\partial \bar{x}}\left(\bar{K}(\bar{T})\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}}\right) = \bar{\rho}\bar{C}(\bar{T})\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{t}} \qquad \text{in } 0<\bar{x}<\bar{L} \tag{2.96}$$

$$-\bar{K}(\bar{T})\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} = \bar{q}_l \qquad \text{at } \bar{x}=0 \tag{2.97}$$

$$\bar{T} = \bar{T}_l \qquad \text{at } \bar{x}=\bar{L} \tag{2.98}$$

$$\bar{T}(\bar{x},\bar{t}) = \bar{T}_0 \qquad \text{for } \bar{t}=0 \tag{2.99}$$

Assuming the following dimensionless quantities

$$x = \frac{\bar{x}}{\bar{L}}, \quad T = \frac{\bar{T}}{\bar{T}_r}, \quad T_0 = \frac{\bar{T}_0}{\bar{T}_r}, \quad K = \frac{\bar{K}}{\bar{K}_r}$$
$$t = \frac{\bar{K}_r \bar{t}}{\bar{\rho}\bar{C}_r \bar{L}^2}, \quad q_l = \frac{\bar{L}\bar{q}_l}{\bar{K}_r \bar{T}_r}, \quad C = \frac{\bar{C}}{\bar{C}_r}, \quad T_l = \frac{\bar{T}_l}{\bar{T}_r}$$

we obtain dimensionless form of equations (2.96-2.99) as follows

$$\frac{\partial}{\partial x}\left(K(T)\frac{\partial T(x,t)}{\partial x}\right) = C(T)\frac{\partial T(x,t)}{\partial t} \qquad \text{in } 0 < x < 1 \tag{2.100}$$

$$-K(T)\frac{\partial T(x,t)}{\partial x} = q_l \qquad \text{at } x = 0 \tag{2.101}$$

$$T = T_l \qquad \text{at } x = 1 \tag{2.102}$$

$$T = T_0 \qquad \text{for } t = 0 \tag{2.103}$$

Here the superscript '-' and subscript 'r' denote dimensional and referenced quantities, respectively. The sensitivity functions, adjoint functions and gradient equations for K and C are adopted as follows:

Sensitivity Problem and Search Step Size

The sensitivity function ΔT_K is the change in estimated temperatures at different positions and times due to change ΔK in $K(x,t)$. The sensitivity function ΔT_K is given by:

$$\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \Delta T_K(x,t)}{\partial x}\right) + \frac{\partial}{\partial x}\left(\Delta K(x,t)\frac{\partial T(x,t)}{\partial x}\right) = C\frac{\partial \Delta T_K(x,t)}{\partial x} \qquad \text{for } 0 < \tag{2.104}$$

$$-K(x,t)\frac{\partial \Delta T_K(x,t)}{\partial x} = \Delta K(x,t)\frac{\partial T(x,t)}{\partial x} \qquad \text{for } x = 0 \tag{2.105}$$

$$\Delta T_K(x,t) = 0 \qquad \text{for } x = 1 \tag{2.106}$$

$$\Delta T_K(x,t) = 0 \qquad \text{for } t = 0 \tag{2.107}$$

Sensitivity function ΔT_C is determined from the equation:

$$\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \Delta T_C(x,t)}{\partial x}\right) = C\frac{\partial \Delta T_C(x,t)}{\partial x} + \Delta C(x,t)\frac{\partial T(x,t)}{\partial x} \qquad \text{for } 0 < x < 1 \tag{2.108}$$

$$\frac{\partial \Delta T_C(x,t)}{\partial x} = 0 \qquad \text{for } x = 0 \tag{2.109}$$

$$\Delta T_C(x,t) = 0 \qquad \text{for } x = 1 \tag{2.110}$$

$$\Delta T_C(x,t) = 0 \quad \text{for } t = 0 \tag{2.111}$$

The objective function can be written as before:

$$J[K(T), C(T)] \equiv J[K(x,t), C(x,t)] = \int_{t=0}^{t_f} \sum_{i=1}^{m} [T_i(x_i,t) - Y_i(x_i,t)]^2 dt \tag{2.112}$$

where, $Y_i(x_i, t)$ is the temperature reading taken with a sensor placed at $x = x_i$ at time t. M sensors are used to record the temperature history over time t_f. Once again, all the sensors are assumed be uniformly placed.

The following iterative process based on the conjugate gradient method is proposed to update K and C:

$$\hat{K}^{n+1}(x,t) = \hat{K}^n(x,t) - \beta_K^n P_K^n(x,t) \tag{2.113}$$

$$\hat{C}^{n+1}(x,t) = \hat{C}^n(x,t) - \beta_C^n P_C^n(x,t) \tag{2.114}$$

The directions of descent for K and C are as follows:

$$P_K^n(x,t) = J'^n_K(x,t) + \nu_K^n P_K^{n-1}(x,t) \tag{2.115}$$

$$P_C^n(x,t) = J'^n_C(x,t) + \nu_C^n P_C^{n-1}(x,t) \tag{2.116}$$

The sensitivity coefficients for K and C are given by

$$\nu_K^n = \frac{\int_{t=0}^{t_f} \int_{x=0}^{1} (J'^n_K)^2 dx dt}{\int_{t=0}^{t_f} \int_{x=0}^{1} (J'^{n-1}_K)^2 dx dt} \tag{2.117}$$

$$\nu_C^n = \frac{\int_{t=0}^{t_f} \int_{x=0}^{1} (J'^n_C)^2 dx dt}{\int_{t=0}^{t_f} \int_{x=0}^{1} (J'^{n-1}_C)^2 dx dt} \tag{2.118}$$

Adjoint Problem and Gradient Equation

To derive the adjoint problem for $K(x,t)$, Equation (2.100) is multiplied by the Lagrange multiplier $\lambda(x,t)$ and the resulting expression is integrated over the time and space domains. Then the result is added to the right-hand side of Equation (2.112). Hence the

esulting expression of the functional $J[K(x,t), C(x,t)]$ becomes

$$J[K(x,t), C(x,t)] = \int_{t=0}^{t_f} \int_{x=0}^{1} \lambda \left[\frac{\partial}{\partial x} \left(K(T) \frac{\partial T(x,t)}{\partial x} \right) - C(T) \frac{\partial T(x,t)}{\partial t} \right] dxdt$$

$$+ \int_{t=0}^{t_f} \sum_{i=1}^{m} [T_i(x_i,t) - Y_i(x_i,t)]^2 dt \qquad (2.119)$$

The variation ΔJ_K is obtained by perturbing T by ΔT_K in Equation (2.119), subtracting from the resulting expression the original Equation (2.119) and neglecting the higher-order terms. We thus obtain

$$\Delta J_K = \int_{t=0}^{t_f} \int_{x=0}^{1} \lambda \left[\frac{\partial}{\partial x} \left(K(x,t) \frac{\partial(\Delta T_K)}{\partial x} \right) + \frac{\partial}{\partial x} \left(\Delta K \frac{\partial T}{\partial x} \right) - C \frac{\partial \Delta T_K}{\partial t} \right] dxdt$$

$$+2 \int_{t=0}^{t_f} \int_{x=0}^{1} \sum_{i=1}^{m} [T - Y] \Delta T_K \delta(x - x_i) dxdt \qquad (2.120)$$

Or $\Delta J_K =$

$$\int_{t=0}^{t_f} \left[\lambda K(x,t) \frac{\partial(\Delta T_K)}{\partial x} \right]_{x=0}^{1} dt - \int_{t=0}^{t_f} \int_{x=0}^{1} K(x,t) \frac{\partial \lambda}{\partial x} \left[\frac{\partial(\Delta T_K)}{\partial x} \right] dxdt$$

$$+ \int_{t=0}^{t_f} \left[\lambda \Delta K \frac{\partial T}{\partial x} \right]_{x=0}^{1} dt - \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta K \left[\frac{\partial \lambda}{\partial x} \frac{\partial T}{\partial x} \right] dxdt$$

$$- \int_{x=0}^{1} [C \lambda \Delta T_K]_{t=0}^{t_f} dx + \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta T_K \frac{\partial(C\lambda)}{\partial t} dxdt$$

$$+ \; 2 \int_{t=0}^{t_f} [(T - Y) \Delta T_K]_{x=1} dt + 2 \int_{t=0}^{t_f} [(T - Y) \Delta T_K]_{x=0} dt$$

$$+ \; 2 \int_{t=0}^{t_f} \int_{x=0}^{1} \sum_{i=2}^{M-1} [T - Y] \Delta T_K \delta(x - x_i) dxdt$$

Or $\Delta J_K =$

$$\int_{t=0}^{1} \left[\lambda K(x,t) \frac{\partial(\Delta T_K)}{\partial x} \right]_{x=0}^{1} dt + \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta T_K \left[\frac{\partial}{\partial x} \left(K(x,t) \frac{\partial \lambda}{\partial x} \right) \right] dxdt$$

$$- \int_{t=0}^{t_f} \left[\Delta T_K K(x,t)\frac{\partial \lambda}{\partial x}\right]_{x=0}^{1} dt + \int_{t=0}^{t_f} \left[\lambda \Delta K \frac{\partial T}{\partial x}\right]_{x=0}^{1} dt - \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta K \left[\frac{\partial \lambda}{\partial x}\frac{\partial T}{\partial x}\right] dxdt$$
$$- \int_{x=0}^{1} [C\lambda \Delta T_K]_{t=0}^{t_f} dx + \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta T_K \frac{\partial (C\lambda)}{\partial t} dxdt + 2\int_{t=0}^{t_f} [(T-Y)\Delta T_K]_{x=1} dt$$
$$+ \; 2\int_{t=0}^{t_f} [(T-Y)\Delta T_K]_{x=0} dt + 2\int_{t=0}^{t_f}\int_{x=0}^{1} \sum_{i=2}^{M-1} [T-Y]\Delta T_K \delta(x-x_i) dxdt$$

Or $\Delta J_K =$

$$\int_{t=0}^{t_f}\int_{x=0}^{1} \Delta T_K \left[\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \lambda}{\partial x}\right) + \frac{\partial (C\lambda)}{\partial t} + 2\sum_{i=2}^{M-1}[T-Y]\delta(x-x_i)\right] dxdt$$
$$+ \int_{t=0}^{t_f} \Delta T_K \left[K(x,t)\frac{\partial \lambda}{\partial x} + 2(T-Y)\right]_{x=0} dt - \int_{t=0}^{t_f} \Delta T_K \left[K(x,t)\frac{\partial \lambda}{\partial x} - 2(T-Y)\right]_{x=1} dt$$
$$- \int_{x=0}^{1} [C\lambda \Delta T_K]_{t=0}^{t_f} dx + \int_{t=0}^{1} \lambda \left[K(x,t)\frac{\partial (\Delta T_K)}{\partial x} + \Delta K \frac{\partial T}{\partial x}\right]_{x=0}^{1} dt$$
$$- \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta K \left[\frac{\partial \lambda}{\partial x}\frac{\partial T}{\partial x}\right] dxdt \tag{2.121}$$

From the sensitivity problem at the two boundaries we get

$$K(x,t)\frac{\partial (\Delta T_K)}{\partial x} + \Delta K \frac{\partial T}{\partial x} = 0 \tag{2.122}$$

As stated earlier, ΔJ_K is not a function ΔT_K. Therefore the integrands containing ΔT_K should be zero. Hence

$$\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial \lambda}{\partial x}\right) + \frac{\partial (C\lambda)}{\partial t} + 2\sum_{i=2}^{M-1}[T-Y]\delta(x-x_i) = 0 \tag{2.123}$$

$$K(x,t)\frac{\partial \lambda}{\partial x} + 2(T-Y) = 0 \qquad \text{at} \quad x = 0 \tag{2.124}$$

$$\lambda = 0 \qquad \text{at} \quad x = 1 \tag{2.125}$$

$$\lambda = 0 \qquad \text{at} \quad t = t_f \tag{2.126}$$

'he Equation (2.121) reduces to

$$\Delta J_K = -\int_{t=0}^{t_f}\int_{x=0}^{1} \Delta K \left[\frac{\partial\lambda}{\partial x}\frac{\partial T}{\partial x}\right] dx dt \tag{2.127}$$

3y definition

$$\Delta J_K = \int_{t=0}^{t_f}\int_{x=0}^{1} J'_K \, dx \, dt \tag{2.128}$$

Comparing the Equations (2.127) and (2.128) we get

$$J'_K = -\frac{\partial\lambda}{\partial x}\frac{\partial T}{\partial x} \tag{2.129}$$

Similarly, considering the variation of C, we obtain the following expression for the gra-
lient of the functional with respect to C:

$$J'_C = -\lambda\frac{\partial T}{\partial x} \tag{2.130}$$

The gradient search procedure for obtaining the property functions K and C can be constructed as follows:

1. Assume the properties $K(x,t)$ and $C(x,t)$; In the absence of additional information, they can be treated as constants.

2. Generate the corresponding temperature field $T(x,t)$, by solving Equations (2.100-2.103).

3. Solve the adjoint problem, Equations (2.123-2.126), and obtain adjoint variable $\lambda(x,t)$.

4. Compute J'_K and J'_C from Equations (2.129) and (2.130)

5. Calculate the conjugate coefficients ν_K and ν_C using Equations (2.117) and (2.118) respectively.

6. Estimate the directions of descent P_K and P_C from Equations (2.115) and (2.116) respectively.

7. Solve the sensitivity problem, Equations (2.104- 2.107) and (2.108-2.111) to obtain sensitivity functions, ΔT_K and ΔT_C.

8. Compute step sizes β_K and β_C using Equations (2.73-2.74).

9. Estimate K and C using Equations (2.113-2.114).

10. Repeat the above calculation procedure until the discrepancy principle given by Equation (2.36) is satisfied.

In summary, the change from flux-flux to flux-temperature boundary conditions leads to the following difficulties:

1. In case of flux-flux boundary conditions, the direct problem is always unsteady whereas it becomes steady a after certain time for flux-temperature boundary conditions.

2. The adjoint function becomes zero at the boundary with the fixed temperature. This can affect the inverse solution.

2.4 Coupled Equations without Source Term

The inverse procedure for two inter-dependent space variables is developed in the present section. For definiteness, the source terms have been set to zero. Inversion of data with source terms is considered in Section 2.5.

2.4.1 Steady State Problem

Direct Problem

Consider the following set of coupled equations for state variables T_1 and T_2 properties K_1 and K_2:

$$\frac{d}{dx}\left(K_1(T_1, T_2)\frac{dT_1(x)}{dx}\right) = 0 \tag{2.131}$$

$$\frac{d}{dx}\left(K_2(T_1, T_2)\frac{dT_2(x)}{dx}\right) = 0 \tag{2.132}$$

$$-K_1 \frac{dT_1}{dx} = q_1 \qquad \text{at } x = 0 \tag{2.133}$$

$$-K_2 \frac{dT_2}{dx} = q_2 \qquad \text{at } x = 0 \tag{2.134}$$

$$T_1(x) = T_{1r}, \quad T_2(x) = T_{2r} \qquad \text{at } x = 1 \tag{2.135}$$

Inverse Problem

For the inverse problem, $K_1(T_1, T_2)$ and $K_2(T_1, T_2)$ are regarded as being unknown, but everything else in equations (2.131-2.132) is known. The experimental values of T_1 and T_2 at some appropriate locations are considered available. The solution of the inverse problem is to be obtained in such a way that the following functional is minimized:

$$J[K_1, K_2] \equiv J[K_1(x), K_2(x)] = \sum_{i=1}^{M} [T_1(x_i) - Y_1(x_i)]^2$$

$$+ \sum_{i=1}^{M} [T_2(x_i) - Y_2(x_i)]^2 \tag{2.136}$$

where $Y_1(x_i)$ and $Y_2(x_i)$ are experimental values of $T_1(x_i)$ and $T_2(x_i)$ respectively.

Conjugate Gradient Method for Minimization

The following iterative process based on the conjugate gradient method is used for estimation of $K_1(x)$ and $K_2(x)$ by minimizing the above functional $J[K_1(x), K_2(x)]$

$$K_1^{n+1}(x) = K_1^n(x) - \beta_{K1}^n P_{K1}^n(x) \tag{2.137}$$

$$K_2^{n+1}(x) = K_2^n(x) - \beta_{K2}^n P_{K2}^n(x) \tag{2.138}$$

where β_{K1}^n, β_{K2}^n are step sizes for K_1 and K_2 in going from nth to $(n+1)$th iteration. The directions of descent, P_{K1}^n and P_{K1}^n for K_1 and K_2 are given by

$$P_{K1}^n(x) = J'^n_{K1}(x) + \nu_{K1}^n P_{K1}^{n-1}(x) \tag{2.139}$$

$$P^n_{K2}(x) = J'^n_{K2}(x) + \nu^n_{K2} P^{n-1}_{K2}(x) \tag{2.140}$$

These are the conjugation of the gradient directions J'^n_{K1} and J'^n_{K1} at iteration n and the directions of descent P^{n-1}_{K1} and P^{n-1}_{K2} at iteration $n-1$ for K_1 and K_2 respectively. The conjugate coefficients are determined from

$$\nu^n_{K1} = \frac{\int x = 0^1 (J'^n_{K1})^2 dx}{\int x = 0^1 (J'^{n-1}_{K1})^2 dx} \qquad \text{with} \quad \nu^0_{K1} = 0 \tag{2.141}$$

$$\nu^n_{K2} = \frac{\int\limits_{x=0}^{1} (J'^n_{K2})^2 dx}{\int\limits_{x=0}^{1} (J'^{n-1}_{K2})^2 dx} \qquad \text{with} \quad \nu^0_{K2} = 0 \tag{2.142}$$

The intermediate steps in the inverse procedure are summarized below:

Sensitivity Problem for K_1

$$\frac{d}{dx}\left[K_1(x)\frac{d(\Delta T_1)_{K1}}{dx}\right] + \frac{d}{dx}\left[\Delta K_1 \frac{dT_1}{dx}\right] = 0 \tag{2.143}$$

$$\frac{d}{dx}\left[K_2(x)\frac{d(\Delta T_2)_{K1}}{dx}\right] = 0 \tag{2.144}$$

$$-K_1\frac{(\Delta T_1)_{K1}}{dx} = \Delta K_1 \frac{dT_1}{dx} \tag{2.145}$$

$$-K_2\frac{(\Delta T_2)_{K1}}{dx} = 0 \tag{2.146}$$

$$(\Delta T_1)_{K1} = 0, \quad (\Delta T_2)_{K1} = 0 \qquad \text{at} \quad x = 1 \tag{2.147}$$

Sensitivity Problem for K_2

$$\frac{d}{dx}\left[K_1(x)\frac{d(\Delta T_1)_{K2}}{dx}\right] = 0 \tag{2.148}$$

$$\frac{d}{dx}\left[K_2(x)\frac{d(\Delta T_2)_{K2}}{dx}\right] + \frac{d}{dx}\left[\Delta K_2 \frac{dT_2}{dx}\right] = 0 \tag{2.149}$$

$$-K_1\frac{(\Delta T_1)_{K2}}{dx} = 0 \quad \text{at} \quad x = 0 \tag{2.150}$$

$$-K_2\frac{(\Delta T_2)_{K2}}{dx} = \Delta K_2 \frac{dT_2}{dx} \quad \text{at} \quad x = 0 \tag{2.151}$$

$$(\Delta T_1)_{K2} = 0, \quad (\Delta T_2)_{K2} = 0 \qquad \text{at} \quad x = 1 \tag{2.152}$$

Step Sizes

The functional $J(K_1^{n+1}, K_2^{n+1})$ for iteration $n+1$ is given by

$$J(K_1^{n+1}, K_2^{n+1}) = \sum_{i=1}^{M}[T_1(K_1^n - \beta_{K1}^n P_{K1}^n, K_2^n - \beta_{K2}^n P_{K2}^n) - Y_1]_i^2$$

$$+ \sum_{i=1}^{M}[T_2(K_1^n - \beta_{K1}^n P_{K1}^n, K_2^n - \beta_{K2}^n P_{K2}^n) - Y_2]_i^2 \qquad (2.153)$$

where K_1^{n+1} and K_2^{n+1} have been replaced by the expressions given by equations (2.137-2.138). Expanding (2.153) using Taylor expansion and neglecting higher-order terms we get

$J(K_1^{n+1}, K_2^{n+1}) =$

$$\sum_{i=1}^{M}\left[T_1(K_1^n, K_2^n) - \beta_{K1}^n\left(P_{K1}^n\frac{\partial T_1}{\partial K_1}\right) - \beta_{K2}^n\left(P_{K2}^n\frac{\partial T_1}{\partial K_2}\right) - Y_1\right]_i^2$$
$$+ \sum_{i=1}^{M}\left[T_2(K_1^n, K_2^n) - \beta_{K1}^n\left(P_{K1}^n\frac{\partial T_2}{\partial K_1}\right) - \beta_{K2}^n\left(P_{K2}^n\frac{\partial T_2}{\partial K_2}\right) - Y_2\right]_i^2$$

Or $J(K_1^{n+1}, K_2^{n+1}) =$

$$\sum_{i=1}^{M}[T_1(K_1^n, K_2^n) - \beta_{K1}^n\Delta(T_1)_{K1}^n - \beta_{K2}^n\Delta(T_1)_{K2}^n - Y_1]_i^2 +$$
$$\sum_{i=1}^{M}[T_2(K_1^n, K_2^n, C^n) - \beta_{K1}^n\Delta(T_2)_{K1}^n - \beta_{K2}^n\Delta(T_2)_{K2}^n - Y_1]_i^2\, dt \qquad (2.154)$$

where $\Delta K_1 = P_{K1}^n$ and $\Delta K_2 = P_{K2}^n$. Now the step sizes β_{K1}^n and β_{K2}^n in such a way that the functional given by the Equation (2.154) is minimized. Therefore

$$\frac{\partial J^{n+1}}{\partial \beta_{K1}^n} = 0 \qquad (2.155)$$

$$\frac{\partial J^{n+1}}{\partial \beta_{K2}^n} = 0 \qquad (2.156)$$

From Equation (2.155) we get

$$\beta_{K1}^n \sum_{i=1}^{M}[(\Delta T_1)_{K1}^2 + (\Delta T_2)_{K1}^2]_{x=xi}$$
$$+ \quad \beta_{K2}^n \sum_{i=1}^{M}[(\Delta T_1)_{K1}(\Delta T_1)_{K2} + (\Delta T_2)_{K1}(\Delta T_2)_{K2}]_{x=xi}$$
$$= \quad \sum_{i=1}^{M}[(T_1 - Y_1)(\Delta T_1)_{K1} + (T_2 - Y_2)(\Delta T_2)_{K1}]_{x=xi} \qquad (2.157)$$

Equation (2.157) can be written as

$$a_{11}\beta_{K1} + a_{12}\beta_{K2} = b_1 \tag{2.158}$$

Similarly, from (2.156) we have

$$a_{21}\beta_{K1} + a_{22}\beta_{K2} = b_2 \tag{2.159}$$

where

$$\begin{aligned}
a_{11} &= \sum_{i=1}^{M}[(\Delta T_1)^2_{K1} + (\Delta T_2)^2_{K1}]_{x=xi} && (2.160)\\
a_{12} &= \sum_{i=1}^{M}[(\Delta T_1)_{K1}(\Delta T_1)_{K2} + (\Delta T_2)_{K1}(\Delta T_2)_{K2}]_{x=xi} && (2.161)\\
b_1 &= \sum_{i=1}^{M}[(T_1 - Y_1)(\Delta T_1)_{K1} + (T_2 - Y_2)(\Delta T_2)_{K1}]_{x=xi} && (2.162)\\
a_{21} &= \sum_{i=1}^{M}[(\Delta T_1)_{K1}(\Delta T_1)_{K2} + (\Delta T_2)_{K1}(\Delta T_2)_{K2}]_{x=xi} && (2.163)\\
a_{22} &= \sum_{i=1}^{M}[(\Delta T_1)^2_{K2} + (\Delta T_2)^2_{K2}]_{x=xi} && (2.164)\\
b_2 &= \sum_{i=1}^{M}[(T_1 - Y_1)(\Delta T_1)_{K2} + (T_2 - Y_2)(\Delta T_2)_{K2}]_{x=xi} && (2.165)
\end{aligned}$$

Adjoint Problem

To derive the adjoint problem for $K_1(x)$ and $K_2(x)$ equations (2.131) and (2.132) are multiplied respectively by the Lagrange multipliers $\lambda_1(x)$ and $\lambda_2(x)$ and the resulting expression is integrated over the space domain. Then the result is added to the right-hand side of equation (2.136) to yield the following expression for the functional $J[K_1(x), K_2(x)]$:

$$\begin{aligned}
J[K_1(x), K_2(x)] &= \int_{x=0}^{1} \lambda_1 \left[\frac{d}{dx}\left(K_1(x)\frac{dT_1(x)}{dx}\right)\right] dx + \int_{x=0}^{1} \lambda_2 \left[\frac{d}{dx}\left(K_2(x)\frac{dT_2(x)}{dx}\right)\right] dx \\
&+ \sum_{i=1}^{M}(T_{1i} - Y_{1i})^2 + \sum_{i=1}^{M}(T_{2i} - Y_{2i})^2
\end{aligned} \tag{2.166}$$

The variation of the functional, ΔJ_{k1} due to change of parameter K_1 to $K_1 + \Delta K_1$ is given by

$$\Delta J_{K1} = \int_{x=0}^{1} \lambda_1 \left[\frac{d}{dx}\left(K_1(x)\frac{d(\Delta T_{K1})}{dx}\right) + \frac{d}{dx}\left(\Delta K_1 \frac{dT_1}{dx}\right)\right] dx$$

$$+ \int_{x=0}^{1} \lambda_2 \left[\frac{d}{dx} \left(K_2(x) \frac{d(\Delta T_2)_{K1}}{dx} \right) \right] dx + 2 \int_{x=0}^{1} \sum_{i=1}^{m} [T_1 - Y_1](\Delta T_1)_{K1} \delta(x - x_i) dx$$
$$+ \; 2 \int_{x=0}^{1} \sum_{i=1}^{m} [T_2 - Y_2](\Delta T_2)_{K1} \delta(x - x_i) dx \qquad (2.167)$$

Or $\Delta J_{K1} =$

$$\left[\lambda_1 K_1(x) \frac{d(\Delta T_1)_{K1}}{dx} \right]_{x=0}^{1} - \int_{x=0}^{1} K_1(x) \frac{d\lambda_1}{dx} \left[\frac{d(\Delta T_1)_{K1}}{dx} \right] dx$$
$$+ \left[\lambda_1 \Delta K_1 \frac{dT_1}{dx} \right]_{x=0}^{1} - \int_{x=0}^{1} \Delta K_1 \left[\frac{d\lambda_1}{dx} \frac{dT_1}{dx} \right] dx$$
$$+ \left[\lambda_2 K_2(x) \frac{d(\Delta T_2)_{K1}}{dx} \right]_{x=0}^{1} - \int_{x=0}^{1} K_2(x) \frac{d\lambda_2}{dx} \left[\frac{d(\Delta T_2)_{K1}}{dx} \right] dx$$
$$+ \; 2[(T_1 - Y_1)(\Delta T_1)_{K1}]_{x=1} + 2[(T_2 - Y_2)(\Delta T_2)_{K1}]_{x=1}$$
$$+ \; 2[(T_1 - Y_1)(\Delta T_1)_{K1}]_{x=0} + 2[(T_2 - Y_2)(\Delta T_2)_{K1}]_{x=0}$$
$$+ \; 2 \int_{x=0}^{1} \sum_{i=2}^{M-1} [T_1 - Y_1](\Delta T_1)_{K1} \delta(x - x_i) dx$$
$$+ \; 2 \int_{x=0}^{1} \sum_{i=2}^{M-1} [T_2 - Y_2](\Delta T_2)_{K1} \delta(x - x_i) dx \qquad (2.168)$$

Or $\Delta J_{K1} =$

$$\left[\lambda_1 K_1(x) \frac{d(\Delta T_1)_{K1}}{dx} \right]_{x=0}^{1} - \left[(\Delta T_1)_{K1} K_1(x) \frac{d\lambda_1}{dx} \right]_{x=0}^{1}$$
$$+ \int_{x=0}^{1} (\Delta T_1)_{K1} \left[\frac{d}{dx} \left(K_1(x) \frac{d\lambda_1}{dx} \right) \right] dx + \left[\lambda_1 \Delta K_1 \frac{dT_1}{dx} \right]_{x=0}^{1}$$
$$- \int_{x=0}^{1} \Delta K_1 \left[\frac{d\lambda_1}{dx} \frac{dT_1}{dx} \right] dx + \left[\lambda_2 K_2(x) \frac{d(\Delta T_2)_{K1}}{dx} \right]_{x=0}^{1}$$
$$- \left[(\Delta T_2)_{K1} K_2(x) \frac{d\lambda_2}{dx} \right]_{x=0}^{1} + \int_{x=0}^{1} (\Delta T_2)_{K1} \left[\frac{d}{dx} \left(K_2(x) \frac{d\lambda_2}{dx} \right) \right] dx$$
$$+ \; 2[(T_1 - Y_1)(\Delta T_1)_{K1}]_{x=1} + 2[(T_2 - Y_2)(\Delta T_2)_{K1}]_{x=1}$$
$$+ \; 2[(T_1 - Y_1)(\Delta T_1)_{K1}]_{x=0} + 2[(T_2 - Y_2)(\Delta T_2)_{K1}]_{x=0}$$
$$+ \; 2 \int_{x=0}^{1} \sum_{i=2}^{M-1} [T_1 - Y_1](\Delta T_1)_{K1} \delta(x - x_i) dx$$
$$+ \; 2 \int_{x=0}^{1} \sum_{i=2}^{M-1} [T_2 - Y_2](\Delta T_2)_{K1} \delta(x - x_i) dx \qquad (2.169)$$

Now we have $(\Delta T_1)_{K1}=(\Delta T_2)_{K1}=0$ at $x = 1$. Thus Equation (2.169) becomes

$$\begin{aligned}
\Delta J_{K1} &= (\Delta T_1)_{K1}\left[K_1\frac{d(\lambda_1)}{dx} + 2(T_1 - Y_1)\right]_{x=0} \\
&+ \int_{x=0}^{1} (\Delta T_1)_{K1}\left[\frac{d}{dx}\left(K_1(x)\frac{d\lambda_1}{dx}\right) + \sum_{i=2}^{M-1}(T_1 - Y_1)\delta(x - x_i)\right] dx \\
&+ \int_{x=0}^{1} (\Delta T_2)_{K1}\left[\frac{d}{dx}\left(K_2(x)\frac{d\lambda_2}{dx}\right) + \sum_{i=2}^{M-1}(T_2 - Y_2)\delta(x - x_i)\right] dx \\
&+ (\Delta T_2)_{K1}\left[K_2\frac{d(\lambda_2)}{dx} + 2(T_2 - Y_2)\right]_{x=0} \\
&+ \left[\lambda_1\left(K_1(x)\frac{d(\Delta T_1)_{K1}}{dx} + \Delta K_1\frac{dT_1}{dx}\right)\right]_{x=0}^{1} \\
&+ \left[\lambda_2 K_2(x)\frac{d(\Delta T_2)_{K1}}{dx}\right]_{x=0}^{1} - \int_{x=0}^{1}\Delta K_1\left[\frac{d\lambda_1}{dx}\frac{dT_1}{dx}\right]dx \qquad (2.170)
\end{aligned}$$

We assume that the values of Lagrange multipliers λ_1 and λ_2 are zero at the two boundaries. Since ΔJ_{K1} does not depend on the variations $(\Delta T_1)_{K1}$ and $(\Delta T_2)_{K1}$, the integrands containing $(\Delta T_1)_{K1}$ and $(\Delta T_2)_{K1}$ are zero. We thus have

$$\frac{d}{dx}\left(K_1(x)\frac{d\lambda_1}{dx}\right) + \sum_{i=2}^{M-1}[T_1 - Y_1]\delta(x - x_i) = 0 \qquad (2.171)$$

$$\frac{d}{dx}\left(K_2(x)\frac{d\lambda_2}{dx}\right) + \sum_{i=2}^{M-1}[T_2 - Y_2]\delta(x - x_i) = 0 \qquad (2.172)$$

$$K_1\frac{d\lambda_1}{dx} + 2(T_1 - Y_1) = 0, \quad \text{at} \quad x = 0 \qquad (2.173)$$

$$K_2\frac{d\lambda_2}{dx} + 2(T_2 - Y_2) = 0, \quad \text{at} \quad x = 0 \qquad (2.174)$$

$$\lambda_1 = \lambda_2 = 0, \quad \text{at} \quad x = 1 \qquad (2.175)$$

Equations (2.171-2.175) can be solved directly to give the adjoint functions λ_1 and λ_2.

Gradient Equations

Using Equations (2.171-2.175) Equation (2.170) can be reduced to

$$\Delta J_{K1} = -\int_{x=0}^{1}\Delta K_1\left[\frac{d\lambda_1}{dx}\frac{dT_1}{dx}\right]dx \qquad (2.176)$$

From the definition of ΔJ_{K1} we have

$$\Delta J_{K1} = \int_{x=0}^{1} J'_{K1}(x)\Delta K_1 dx \tag{2.177}$$

and comparing equations (2.176) and (2.177) we get

$$J'_{K1} = -\frac{d\lambda_1}{dx}\frac{dT_1}{dx} \tag{2.178}$$

Similarly, considering the variation of the objective function due to variation of $K_2(x)$ one can get the following gradient equation

$$J'_{K2} = -\frac{d\lambda_2}{dx}\frac{dT_2}{dx} \tag{2.179}$$

The inverse technique for reconstructing $K_1(T_1, T_2)$ and $K_1(T_1, T_2)$ can be cast in the following algorithmic form:

1. Assume the properties $K_1(x)$ and $K_2(x)$; In the absence of additional information, they can be treated as constants.

2. Generate the corresponding state variables $T_1(x)$ and $T_2(x)$ by solving Equations (2.131-2.135).

3. Solve the adjoint problem, Equations (2.171-2.175), and obtain adjoint variables $\lambda_1(x)$ and $\lambda_2(x)$.

4. Compute J'_{K1} and J'_{K2} from Equations (2.178) and (2.179).

5. Calculate the conjugate coefficients ν_{K1} and ν_{K2} using Equations (2.141) and (2.142) respectively.

6. Estimate the directions of descent P_{K1} and P_{K2} from Equations (2.139) and (2.140) respectively.

7. Solve the sensitivity problem, Equations (2.143- 2.152) to obtain sensitivity functions, ΔT_{1K1}, ΔT_{2K1}, ΔT_{1K2} and ΔT_{2K2}.

8. Compute step sizes β_{K1} and β_{K2} using Equations (2.158-2.159).

9. Estimate K_1 and K_2 using Equations (2.137-2.138).

10. Repeat the above calculation procedure until the discrepancy principle given by Equation (2.36) is satisfied.

2.4.2 Transient Problem

Direct Problem

Consider the system of equations

$$\frac{\partial}{\partial x}\left(K_1(T_1,T_2)\frac{\partial T_1(x,t)}{\partial x}\right) = C(T_1,T_2)\frac{\partial T_1(x,t)}{\partial t} \tag{2.180}$$

$$\frac{\partial}{\partial x}\left(K_2(T_1,T_2)\frac{\partial T_2(x,t)}{\partial x}\right) = C(T_1,T_2)\frac{\partial T_2(x,t)}{\partial t} \tag{2.181}$$

$$-K_1(T_1,T_2)\frac{\partial T_1(x,t)}{\partial x} = q_1 \qquad \text{at } x = 0 \tag{2.182}$$

$$-K_2(T_1,T_2)\frac{\partial T_2(x,t)}{\partial x} = q_2 \qquad \text{at } x = 0 \tag{2.183}$$

$$T_1(x,t) = T_1 l \qquad \text{at } x = 1 \tag{2.184}$$

$$T_2(x,t) = T_2 l \qquad \text{at } x = 1 \tag{2.185}$$

$$T_1(x,t) = T_{10} \qquad \text{for } t = 0 \tag{2.186}$$

$$T_1(x,t) = T_{10} \qquad \text{for } t = 0 \tag{2.187}$$

with K_1, K_2 and C as the undetermined parameters.

Inverse Problem

For the inverse problem, $K_1(T_1,T_2)$, $K_2(T_1,T_2)$ and $C(T_1,T_2)$ are regarded as being unknown, other quantities in Equations (2.180-2.187) being known. The experimental values of T_1 and T_2 at some appropriate locations are considered available. The solution of the inverse problem is to be obtained in such a way that the following functional is minimized:

$$J[K_1,K_2,C] \equiv J[K_1(x,t),K_2(x,t),C(x,t)] = \int_{t=0}^{t_f}\sum_{i=1}^{M}[T_1(x_i,t) - Y_1(x_i,t)]^2 dt$$

$$+\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_2(x_i,t) - Y_2(x_i,t)]^2 dt \tag{2.188}$$

where $Y_1(x_i,t)$ and $Y_2(x_i,t)$ are experimental values of $T_1(x_i,t)$ and $T_2(x_i,t)$ respectively.

Conjugate Gradient Method for Minimization

The following iterative process based on the conjugate gradient method is used for estimation of $K_1(x,t)$, $K_2(x,t)$ and $C(x,t)$ by minimizing the above functional $J[K_1(x,t), K_2(x,t), C(x,t)]$

$$K_1^{n+1}(x,t) = K_1^n(x,t) - \beta_{K1}^n P_{K1}^n(x,t) \tag{2.189}$$

$$K_2^{n+1}(x,t) = K_2^n(x,t) - \beta_{K2}^n P_{K2}^n(x,t) \tag{2.190}$$

$$C^{n+1}(x,t) = C^n(x,t) - \beta_C^n P_C^n(x,t) \tag{2.191}$$

where $\beta_{K1}^n(x,t)$, $\beta_{K2}^n(x,t)$ and $\beta_C^n(x,t)$ are step sizes for K_1, K_2 and C in going from the nth to $(n+1)th$ iteration. The directions of descent, P_{K1}^n, P_{K1}^n, P_C^n, for K_1, K_2 and C are given by

$$P_{K1}^n(x,t) = J'^n_{K1}(x,t) + \nu_{K1}^n P_{K1}^{n-1}(x,t) \tag{2.192}$$

$$P_{K2}^n(x,t) = J'^n_{K2}(x,t) + \nu_{K2}^n P_{K2}^{n-1}(x,t) \tag{2.193}$$

$$P_C^n(x,t) = J'^n_C(x,t) + \nu_C^n P_C^{n-1}(x,t) \tag{2.194}$$

These are the conjugation of the gradient directions J'^n_{K1}, J'^n_{K1} and J'^n_C at iteration n and the directions of descent P_{K1}^{n-1}, P_{K2}^{n-1} and P_C^{n-1} at iteration $n-1$ for K_1, K_2 and C respectively. The conjugate coefficients are determined from

$$\nu_{K1}^n = \frac{\int_{x=0}^1 (J'^n_{K1})^2 dx}{\int_{x=0}^1 (J'^{n-1}_{K1})^2 dx} \qquad \text{with} \quad \nu_{K1}^0 = 0 \tag{2.195}$$

$$\nu_{K2}^n = \frac{\int_{x=0}^1 (J'^n_{K2})^2 dx}{\int_{x=0}^1 (J'^{n-1}_{K2})^2 dx} \qquad \text{with} \quad \nu_{K2}^0 = 0 \tag{2.196}$$

$$\nu_C^n = \frac{\int_{x=0}^1 (J'^n_C)^2 dx}{\int_{x=0}^1 (J'^{n-1}_C)^2 dx} \qquad \text{with} \quad \nu_C^0 = 0 \tag{2.197}$$

Sensitivity Problem and Step Size

There are three unknown parameters K_1, K_2 and C which are to be determined. In order to derive the sensitivity problem for each unknown, we should perturb the unknowns are perturbed one at a time.

Sensitivity Problem for K_1

It is assumed that when $K_1(x,t)$ undergoes a variation ΔK_1, $T_1(x,t)$ and $T_2(x,t)$ are perturbed by $T_1 + \Delta T_1$ and $T_2 + \Delta T_2$ respectively. Then replacing K_1 by $K + K_1$, T_1 by $T_1 + (\Delta T_1)_{K1}$ and T_2 by $T_2 + (\Delta T_2)_{K1}$ in the direct problem, and subtracting from the resulting expressions and neglecting the higher-order terms, the following sensitivity functions $(\Delta T_1)_{K1}$ and $(\Delta T_2)_{K1}$ are obtained.

$$\frac{\partial}{\partial x}\left[K_1 \frac{\partial(\Delta T_1)_{K1}}{\partial x}\right] + \frac{\partial}{\partial x}\left[\Delta K_1 \frac{\partial T_1}{\partial x}\right] = C\frac{\partial(\Delta T_1)_{K1}}{\partial t} \tag{2.198}$$

$$\frac{\partial}{\partial x}\left[K_2 \frac{\partial(\Delta T_2)_{K1}}{\partial x}\right] = C\frac{\partial(\Delta T_2)_{K1}}{\partial t} \tag{2.199}$$

$$K_1 \frac{\partial(\Delta T_1)_{K1}}{\partial x} + \Delta K_1 \frac{\partial T_1}{\partial x} = 0 \qquad \text{at} \quad x = 0 \tag{2.200}$$

$$K_2 \frac{\partial(\Delta T_2)_{K1}}{\partial x} = 0 \qquad \text{at} \quad x = 0 \tag{2.201}$$

$$(\Delta T_1)_{K1} = 0 \qquad \text{and} \qquad (\Delta T_2)_{K1} = 0 \qquad \text{at} \quad x = 1 \tag{2.202}$$

$$(\Delta T_1)_{K1} = 0 \qquad \text{and} \qquad (\Delta T_2)_{K1} = 0 \qquad \text{at} \quad t = 0 \tag{2.203}$$

Sensitivity Problem for K_2

Following an identical procedure in deriving the sensitivity functions for K_1 we get the sensitivity problem for K_2 as follows

$$\frac{\partial}{\partial x}\left[K_1 \frac{\partial(\Delta T_1)_{K2}}{\partial x}\right] = C\frac{\partial(\Delta T_1)_{K2}}{\partial t} \tag{2.204}$$

$$\frac{\partial}{\partial x}\left[K_2 \frac{\partial(\Delta T_2)_{K2}}{\partial x}\right] + \frac{\partial}{\partial x}\left[\Delta K_2 \frac{\partial T_2}{\partial x}\right] = C\frac{\partial(\Delta T_2)_{K2}}{\partial t} \tag{2.205}$$

$$K_1 \frac{\partial(\Delta T_1)_{K2}}{\partial x} = 0 \qquad \text{at} \quad x = 0 \tag{2.206}$$

$$K_2 \frac{\partial(\Delta T_2)_{K2}}{\partial x} + \Delta K_2 \frac{\partial T_2}{\partial x} = 0 \qquad \text{at} \quad x = 0 \tag{2.207}$$

$$(\Delta T_1)_{K2} = 0 \qquad \text{and} \qquad (\Delta T_2)_{K2} = 0 \qquad \text{at} \quad x = 1 \tag{2.208}$$

$$(\Delta T_1)_{K2} = 0 \qquad \text{and} \qquad (\Delta T_2)_{K2} = 0 \qquad \text{at} \quad t = 0 \tag{2.209}$$

Sensitivity Problem for C

The sensitivity functions $(\Delta T_1)_C$ and $(\Delta T_2)_C$ derived as

$$\frac{\partial}{\partial x}\left[K_1\frac{\partial(\Delta T_1)_C}{\partial x}\right] = C\frac{\partial(\Delta T_1)_C}{\partial t} + \Delta C\frac{\partial T_1}{\partial t} \tag{2.210}$$

$$\frac{\partial}{\partial x}\left[K_2\frac{\partial(\Delta T_2)_C}{\partial x}\right] = C\frac{\partial(\Delta T_2)_C}{\partial t} + \Delta C\frac{\partial T_2}{\partial t} \tag{2.211}$$

$$K_1\frac{\partial(\Delta T_1)_C}{\partial x} = 0 \qquad \text{at} \quad x = 0 \tag{2.212}$$

$$K_2\frac{\partial(\Delta T_2)_C}{\partial x} = 0 \qquad \text{at} \quad x = 0 \tag{2.213}$$

$$(\Delta T_1)_C = 0 \qquad \text{and} \qquad (\Delta T_2)_C = 0 \qquad \text{at} \quad x = 1 \tag{2.214}$$

$$(\Delta T_1)_C = 0 \qquad \text{and} \qquad (\Delta T_2)_C = 0 \qquad \text{at} \quad t = 0 \tag{2.215}$$

Step Sizes

The functional $J(K_1^{n+1}, K_2^{n+1}, C^{n+1})$ for iteration $n+1$ is given by

$$J(K_1^{n+1}, K_2^{n+1}, C^{n+1}) = \int_{t=0}^{t_f}\sum_{i=1}^{M}[T_1(K_1^n - \beta_{K1}^n P_{K1}^n, K_2^n - \beta_{K2}^n P_{K2}^n, C^n - \beta_C^n P_C^n) - Y_1]_i^2 dt$$

$$+\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_1(K_1^n - \beta_{K1}^n P_{K1}^n, K_2^n - \beta_{K2}^n P_{K2}^n, C^n - \beta_C^n P_C^n) - Y_1]_i^2 dt \tag{2.216}$$

where K_1^{n+1}, K_2^{n+1} and C^{n+1} have been replaced by the expressions given by equations (2.189-2.191). Expanding (2.216) using Taylor expansion and neglecting higher-order terms we get

$J(K_1^{n+1}, K_2^{n+1}, C^{n+1}) =$

$$\int_{t=0}^{t_f}\sum_{i=1}^{M}\left[T_1(K_1^n, K_2^n, C^n) - \beta_{K1}^n\left(P_{K1}^n\frac{\partial T_1}{\partial K_1}\right) - \beta_{K2}^n\left(P_{K2}^n\frac{\partial T_1}{\partial K_2}\right) - \beta_C^n\left(P_C^n\frac{\partial T_1}{\partial C}\right) - Y_1\right]_i^2 dt$$

$$+\int_{t=0}^{t_f}\sum_{i=1}^{M}\left[T_2(K_1^n, K_2^n, C^n) - \beta_{K1}^n\left(P_{K1}^n\frac{\partial T_2}{\partial K_1}\right) - \beta_{K2}^n\left(P_{K2}^n\frac{\partial T_2}{\partial K_2}\right) - \beta_C^n\left(P_C^n\frac{\partial T_2}{\partial C}\right) - Y_2\right]_i^2 dt$$

Or $J(K_1^{n+1}, K_2^{n+1}, C^{n+1}) =$

$$\int_{t=0}^{t_f} \sum_{i=1}^{M} [T_1(K_1^n, K_2^n, C^n) - \beta_{K1}^n \Delta(T_1)_{K1}^n - \beta_{K2}^n \Delta(T_1)_{K2}^n - \beta_C^n \Delta(T_1)_C^n - Y_1]_i^2 \, dt +$$

$$\int_{t=0}^{t_f} \sum_{i=1}^{M} [T_2(K_1^n, K_2^n, C^n) - \beta_{K1}^n \Delta(T_2)_{K1}^n - \beta_{K2}^n \Delta(T_2)_{K2}^n - \beta_C^n \Delta(T_2)_C^n - Y_1]_i^2 \, dt \quad (2.217)$$

where $\Delta K_1 = P_{K1}^n$, $\Delta K_2 = P_{K2}^n$ and $\Delta C = P_C^n$. Now the step sizes, β_{K1}^n, β_{K2}^n and β_C^n, in such a way that the functional given by the Equation (2.217) is minimized. Therefore

$$\frac{\partial J^{n+1}}{\partial \beta_{K1}^n} = 0 \quad (2.218)$$

$$\frac{\partial J^{n+1}}{\partial \beta_{K2}^n} = 0 \quad (2.219)$$

$$\frac{\partial J^{n+1}}{\partial \beta_C^n} = 0 \quad (2.220)$$

From Equation (2.218) we get

$$\begin{aligned}
& \beta_{K1}^n \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_{K1}^2 + (\Delta T_2)_{K1}^2]_{x=xi} dt \\
+ \; & \beta_{K2}^n \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_{K1}(\Delta T_1)_{K2} + (\Delta T_2)_{K1}(\Delta T_2)_{K2}]_{x=xi} dt \\
+ \; & \beta_C^n \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_C(\Delta T_1)_{K1} + (\Delta T_2)_C(\Delta T_2)_{K1}]_{x=xi} dt \\
= \; & \int_{t=0}^{t_f} \sum_{i=1}^{M} [(T_1 - Y_1)(\Delta T_1)_{K1} + (T_2 - Y_2)(\Delta T_2)_{K1}]_{x=xi} dt
\end{aligned} \quad (2.221)$$

Equation (2.221) can be written as

$$a_{11}\beta_{K1} + a_{12}\beta_{K2} + a_{13}\beta_C = c_1 \quad (2.222)$$

Similarly, from (2.219) and (2.220) we have

$$a_{21}\beta_{K1} + a_{22}\beta_{K2} + a_{23}\beta_C = c_2 \quad (2.223)$$

$$a_{31}\beta_{K1} + a_{32}\beta_{K2} + a_{33}\beta_C = c_3 \tag{2.224}$$

where

$$a_{11} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)^2_{K1} + (\Delta T_2)^2_{K1}]_{x=xi} dt \tag{2.225}$$

$$a_{12} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_{K1}(\Delta T_1)_{K2} + (\Delta T_2)_{K1}(\Delta T_2)_{K2}]_{x=xi} dt \tag{2.226}$$

$$a_{13} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_{K1}(\Delta T_1)_C + (\Delta T_2)_{K1}(\Delta T_2)_C]_{x=xi} dt \tag{2.227}$$

$$c_1 = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(T_1 - Y_1)(\Delta T_1)_{K1} + (T_2 - Y_2)(\Delta T_2)_{K1}]_{x=xi} dt \tag{2.228}$$

$$a_{21} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_{K1}(\Delta T_1)_{K2} + (\Delta T_2)_{K1}(\Delta T_2)_{K2}]_{x=xi} dt \tag{2.229}$$

$$a_{22} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)^2_{K2} + (\Delta T_2)^2_{K2}]_{x=xi} dt \tag{2.230}$$

$$a_{23} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_{K2}(\Delta T_1)_C + (\Delta T_2)_{K2}(\Delta T_2)_C]_{x=xi} dt \tag{2.231}$$

$$c_2 = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(T_1 - Y_1)(\Delta T_1)_{K2} + (T_2 - Y_2)(\Delta T_2)_{K2}]_{x=xi} dt \tag{2.232}$$

$$a_{31} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_{K1}(\Delta T_1)_C + (\Delta T_2)_{K1}(\Delta T_2)_C]_{x=xi} dt \tag{2.233}$$

$$a_{32} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)_{K2}(\Delta T_1)_C + (\Delta T_2)_{K2}(\Delta T_2)_C]_{x=xi} dt \tag{2.234}$$

$$a_{33} = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(\Delta T_1)^2_C + (\Delta T_2)^2_C]_{x=xi} dt \tag{2.235}$$

$$c_3 = \int_{t=0}^{t_f} \sum_{i=1}^{M} [(T_1 - Y_1)(\Delta T_1)_C + (T_2 - Y_2)(\Delta T_2)_C]_{x=xi} dt \tag{2.236}$$

Solving Equations (2.222-2.224) simultaneously we get step sizes β_{K1}, β_{K2} and β_c.

Adjoint Problem and Gradient Equations

To derive the adjoint problem, Equation (2.180) is multiplied by the adjoint function $\lambda_1(x,t)$ and Equation (2.181) is multiplied by $\lambda_2(x,t)$. The resulting expression is integrated over the space and time domains. Then the result is added to the right hand side of Equation (2.188). Then the objective function becomes

$$\begin{aligned} J[K_1, K_2, C] \equiv\ & J[K_1(x,t), K_2(x,t), C(x,t)] = \int_{t=0}^{t_f} \sum_{i=1}^{M} [T_1(x_i,t) - Y_1(x_i,t)]^2 dt \\ &+ \int_{t=0}^{t_f} \sum_{i=1}^{M} [T_2(x_i,t) - Y_2(x_i,t)]^2 dt \\ &+ \int_{t=0}^{t_f} \int_{x=0}^{1} \lambda_1 \left[\frac{\partial}{\partial x}\left(K_1 \frac{\partial T_1(x,t)}{\partial x}\right) - C\frac{\partial T_1(x,t)}{\partial t} \right] dx dt \\ &+ \int_{t=0}^{t_f} \int_{x=0}^{1} \lambda_2 \left[\frac{\partial}{\partial x}\left(K_2 \frac{\partial T_2(x,t)}{\partial x}\right) - C\frac{\partial T_2(x,t)}{\partial t} \right] dx dt \end{aligned} \tag{2.237}$$

The variation ΔJ_{K1} is obtained by perturbing T_1 by $(\Delta T_1)_{K1}$ and T_2 by $(\Delta T_2)_{K2}$ in Equation (2.237). Then the original Equation (2.237) is subtracted from the resulting equation. After neglecting the higher-order terms we get the following expression of the variation ΔJ_{K1}:

$$\begin{aligned} \Delta J_{K1} =\ & 2\int_{t=0}^{t_f} \sum_{i=1}^{M} [T_1(x_i,t) - Y_1(x_i,t)](\Delta T_1)_{K1} dt + 2\int_{t=0}^{t_f} \sum_{i=1}^{M} [T_2(x_i,t) - Y_2(x_i,t)](\Delta T_2)_{K1} dt \\ &+ \int_{t=0}^{t_f} \int_{x=0}^{1} \lambda_1 \left[\frac{\partial}{\partial x}\left(K_1 \frac{\partial (\Delta T_1)_{K1}}{\partial x}\right) + \frac{\partial}{\partial x}\left(\Delta K_1 \frac{\partial T_1}{\partial x}\right) - C\frac{\partial (\Delta T_1)_{K1}}{\partial t} \right] dx dt \\ &+ \int_{t=0}^{t_f} \int_{x=0}^{1} \lambda_2 \left[\frac{\partial}{\partial x}\left(K_2 \frac{\partial (\Delta T_2)_{K1}}{\partial x}\right) - C\frac{\partial (\Delta T_2)_{K1}}{\partial t} \right] dx dt \end{aligned} \tag{2.238}$$

Or $\Delta J_{K1} =$

$$\begin{aligned} & \int_{t=0}^{1} \left[\lambda_1 K_1 \frac{\partial (\Delta T_1)_{K1}}{\partial x} \right]_{x=0}^{1} dt + \int_{t=0}^{t_f} \int_{x=0}^{1} (\Delta T_1)_{K1} \left[\frac{\partial}{\partial x}\left(K_1 \frac{\partial \lambda_1}{\partial x}\right)\right] dx dt \\ - & \int_{t=0}^{t_f} \left[(\Delta T_1)_{K1} K_1 \frac{\partial \lambda_1}{\partial x} \right]_{x=0}^{1} dt + \int_{t=0}^{t_f} \left[\lambda_1 \Delta K_1 \frac{\partial T_1}{\partial x} \right]_{x=0}^{1} dt - \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta K_1 \left[\frac{\partial \lambda_1}{\partial x} \frac{\partial T_1}{\partial x} \right] dx dt \end{aligned}$$

$$
\begin{aligned}
& - \int_{x=0}^{1} [C\lambda_1(\Delta T_1)_{K1}]_{t=0}^{t_f} dx + \int_{t=0}^{t_f}\int_{x=0}^{1} (\Delta T_1)_{K1} \frac{\partial(C\lambda_1)}{\partial t} dxdt \\
& + \int_{t=0}^{1} \left[\lambda_2 K_2 \frac{\partial(\Delta T_2)_{K1}}{\partial x}\right]_{x=0}^{1} dt + \int_{t=0}^{t_f}\int_{x=0}^{1} (\Delta T_2)_{K1} \left[\frac{\partial}{\partial x}\left(K_2 \frac{\partial \lambda_2}{\partial x}\right)\right] dxdt \\
& - \int_{t=0}^{t_f} \left[(\Delta T_2)_{K1} K_2 \frac{\partial \lambda_2}{\partial x}\right]_{x=0}^{1} dt - \int_{x=0}^{1} [C\lambda_2(\Delta T_2)_{K1}]_{t=0}^{t_f} dx \\
& + \int_{t=0}^{t_f}\int_{x=0}^{1} (\Delta T_2)_{K1} \frac{\partial(C\lambda_2)}{\partial t} dxdt + 2\int_{t=0}^{t_f} [(T_1 - Y_1)(\Delta T_1)_{K1}]_{x=0} \\
& + 2\int_{t=0}^{t_f} [(T_1 - Y_1)(\Delta T_1)_{K1}]_{x=1} + 2\int_{t=0}^{t_f}\int_{x=0} \sum_{i=2}^{M} [T_1 - Y_1]\delta(x - x_i)(\Delta T_1)_{K1} dxdt \\
& + 2\int_{t=0}^{t_f} [(T_2 - Y_2)(\Delta T_2)_{K1}]_{x=0} + 2\int_{t=0}^{t_f} [(T_2 - Y_2)(\Delta T_2)_{K1}]_{x=1} \\
& + 2\int_{t=0}^{t_f}\int_{x=0} \sum_{i=2}^{M} [T_2 - Y_2]\delta(x - x_i)(\Delta T_2)_{K1} dxdt \qquad (2.239)
\end{aligned}
$$

Or $\Delta J_{K_1} =$

$$
\begin{aligned}
& \int_{t=0}^{t_f}\int_{x=0}^{1} (\Delta T_1)_{K1} \left[\frac{\partial}{\partial x}\left(K_1 \frac{\partial \lambda_1}{\partial x}\right) + \frac{\partial(C\lambda_1)}{\partial t} + 2\sum_{i=2}^{M-1} [T_1 - Y_1]\delta(x - x_i)\right] dxdt \\
& + \int_{t=0}^{t_f} (\Delta T_1)_{K1} \left[K_1 \frac{\partial \lambda_1}{\partial x} + 2(T_1 - Y_1)\right]_{x=0} dt - \int_{t=0}^{t_f} (\Delta T_1)_{K1} \left[K_1 \frac{\partial \lambda_1}{\partial x} - 2(T_1 - Y_1)\right]_{x=1} dt \\
& - \int_{x=0}^{1} [C\lambda_1(\Delta T_1)_{K1}]_{t=0}^{t_f} dx + \int_{t=0}^{1} \lambda_1 \left[K_1 \frac{\partial(\Delta T_1)_{K1}}{\partial x} + \Delta K_1 \frac{\partial T_1}{\partial x}\right]_{x=0}^{1} dt \\
& + \int_{t=0}^{t_f}\int_{x=0}^{1} (\Delta T_2)_{K1} \left[\frac{\partial}{\partial x}\left(K_2 \frac{\partial \lambda_2}{\partial x}\right) + \frac{\partial(C\lambda_2)}{\partial t} + 2\sum_{i=2}^{M-1} [T_2 - Y_2]\delta(x - x_i)\right] dxdt \\
& + \int_{t=0}^{t_f} (\Delta T_2)_{K1} \left[K2 \frac{\partial \lambda_2}{\partial x} + 2(T_2 - Y_2)\right]_{x=0} dt - \int_{t=0}^{t_f} (\Delta T_2)_{K1} \left[K_2 \frac{\partial \lambda_2}{\partial x} - 2(T_2 - Y_2)\right]_{x=1} dt \\
& - \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta K_1 \left[\frac{\partial \lambda_1}{\partial x}\frac{\partial T_1}{\partial x}\right] dxdt \qquad (2.240)
\end{aligned}
$$

Now the integrands containing $(\Delta T_1)_{K1}$ and $(\Delta T_1)_{K1}$ should be zero. We thus have

$$\frac{\partial}{\partial x}\left(K_1\frac{\partial \lambda_1}{\partial x}\right) + \frac{\partial (C\lambda_1)}{\partial t} + 2\sum_{i=2}^{M-1}[T_1 - Y_1]\delta(x - x_i) = 0 \tag{2.241}$$

$$K_1\frac{\partial \lambda_1}{\partial x} + 2(T_1 - Y_1) = 0 \qquad \text{for} \quad x = 0 \tag{2.242}$$

$$\lambda_1 = 0 \qquad \text{for} \quad x = 1 \tag{2.243}$$

$$\lambda_1 = 0 \qquad \text{for} \quad t = t_f \tag{2.244}$$

$$\frac{\partial}{\partial x}\left(K_2\frac{\partial \lambda_2}{\partial x}\right) + \frac{\partial (C\lambda_2)}{\partial t} + 2\sum_{i=2}^{M-1}[T_2 - Y_2]\delta(x - x_i) = 0 \tag{2.245}$$

$$K_2\frac{\partial \lambda_2}{\partial x} + 2(T_2 - Y_2) = 0 \qquad \text{for} \quad x = 0 \tag{2.246}$$

$$\lambda_2 = 0 \qquad \text{for} \quad x = 1 \tag{2.247}$$

$$\lambda_2 = 0 \qquad \text{for} \quad t = t_f \tag{2.248}$$

$$\Delta J_{K1} = -\int_{t=0}^{t_f}\int_{x=0}^{1} \Delta K_1 \left[\frac{\partial \lambda_1}{\partial x}\frac{\partial T_1}{\partial x}\right] dxdt \tag{2.249}$$

From the definition of ΔJ_{K1}

$$\Delta J_{K1} = \int_{t=0}^{t_f}\int_{x=0}^{1} J'_{K1}\Delta K_1 dxdt \tag{2.250}$$

Comparing Equations (2.249-2.250) the following gradient equation is obtained

$$J'_{K1}(x,t) = -\frac{\partial \lambda_1}{\partial x}\frac{\partial T_1}{\partial x} \tag{2.251}$$

Considering the variation of K_2 one can show the following relationship

$$J'_{K2}(x,t) = -\frac{\partial \lambda_2}{\partial x}\frac{\partial T_2}{\partial x} \tag{2.252}$$

For deriving the expression for the gradient of the functional with respect to C, we need to apply perturbation principle in Equation (2.237). It is assumed that when $C(x,t)$ undergoes a variation $\Delta C(x,t)$, $T_1(x,t)$ and $T_2(x,t)$ are perturbed by $T_1 + (\Delta T_1)_C$ and $T_2 + (\Delta T_2)_C$. Then replacing C by $C + \Delta C$, T_1 by $T_1 + (\Delta T_1)_C$ and T_2 by $T_2 + (\Delta T_2)_C$ in Equation (2.237), subtracting Equation (2.237) and neglecting the higher-order terms, we get the variation of the functional as follows:

$$\begin{aligned}
\Delta J_C &= 2\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_1(x_i,t) - Y_1(x_i,t)](\Delta T_1)_C dt + 2\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_2(x_i,t) - Y_2(x_i,t)](\Delta T_2)_C dt \\
&+ \int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_1\left[\frac{\partial}{\partial x}\left(K_1\frac{\partial(\Delta T_1)_C}{\partial x}\right) - \Delta C\frac{\partial T_1}{\partial t} - C\frac{\partial(\Delta T_1)_C}{\partial t}\right]dxdt \\
&+ \int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_2\left[\frac{\partial}{\partial x}\left(K_2\frac{\partial(\Delta T_2)_C}{\partial x}\right) - \Delta C\frac{\partial T_2}{\partial t} - C\frac{\partial(\Delta T_2)_C}{\partial t}\right]dxdt
\end{aligned} \tag{2.253}$$

Or $\Delta J_C =$

$$\begin{aligned}
& 2\int_{t=0}^{t_f}[T_1(x_1,t) - Y_1(x_1,t)](\Delta T_1)_C dt + 2\int_{t=0}^{t_f}[T_2(x_1,t) - Y_2(x_1,t)](\Delta T_2)_C dt \\
&+ 2\int_{t=0}^{t_f}[T_1(x_M,t) - Y_1(x_M,t)](\Delta T_1)_C dt + 2\int_{t=0}^{t_f}[T_2(x_M,t) - Y_2(x_M,t)](\Delta T_2)_C dt \\
&+ 2\int_{t=0}^{t_f}\int_{x=0}^{1}\sum_{i=2}^{M-1}[T_1(x,t) - Y_1(x,t)](\Delta T_1)_C\delta(x-x_i)dxdt \\
&+ 2\int_{t=0}^{t_f}\int_{x=0}^{1}\sum_{i=2}^{M-1}[T_2(x,t) - Y_2(x,t)](\Delta T_2)_C\delta(x-x_i)dxdt \\
&+ \int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_1\left[\frac{\partial}{\partial x}\left(K_1\frac{\partial(\Delta T_1)_C}{\partial x}\right) - C\frac{\partial(\Delta T_1)_C}{\partial t}\right]dxdt \\
&+ \int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_2\left[\frac{\partial}{\partial x}\left(K_2\frac{\partial(\Delta T_2)_C}{\partial x}\right) - C\frac{\partial(\Delta T_2)_C}{\partial t}\right]dxdt \\
&- \int_{t=0}^{t_f}\int_{x=0}^{1}\Delta C\left(\lambda_1\frac{\partial T_1}{\partial t} + \lambda_2\frac{\partial T_2}{\partial t}\right)dx\ dt
\end{aligned} \tag{2.254}$$

Or $\Delta J_C =$

$$\int_{t=0}^{t_f}\int_{x=0}^{1}(\Delta T_1)_C\left[\frac{\partial}{\partial x}\left(K_1\frac{\partial\lambda_1}{\partial x}\right) + \frac{\partial(C\lambda_1)}{\partial t} + \sum_{i=2}^{M-1}(T_1 - Y_1)\delta(x-x_i)\right]dxdt$$

$$
\begin{aligned}
&+ \int_{t=0}^{t_f}\int_{x=0}^{1} (\Delta T_2)_C \left[\frac{\partial}{\partial x}\left(K_2\frac{\partial \lambda_2}{\partial x}\right) + \frac{\partial (C\lambda_2)}{\partial t} + \sum_{i=2}^{M-1}(T_2 - Y_2)\delta(x - x_i)\right] dx\; dt \\
&- \int_{t=0}^{t_f}\left[(\Delta T_1)_C\left(K_1\frac{\partial \lambda_1}{\partial x} - 2(T_1 - Y_1)\right)\right]_{x=0} dt \\
&- \int_{t=0}^{t_f}\left[(\Delta T_2)_C\left(K_2\frac{\partial \lambda_2}{\partial x} - 2(T_2 - Y_2)\right)\right]_{x=0} dt \\
&- \int_{t=0}^{t_f}\left[\lambda_1 K_1\frac{\partial (\Delta T_1)_C}{\partial x}\right]_{x=1} dt - \int_{t=0}^{t_f}\left[\lambda_2 K_2\frac{\partial (\Delta T_2)_C}{\partial x}\right]_{x=1} dt \\
&- \int_{x=0}^{1}[\lambda_1 C(\Delta T_1)_C]_{t_f} dx - \int_{x=0}^{1}[\lambda_2 C(\Delta T_2)_C]_{t_f} dx \\
&- \int_{t=0}^{t_f}\int_{x=0}^{1}\Delta C\left(\lambda_1\frac{\partial T_1}{\partial t} + \lambda_2\frac{\partial T_2}{\partial t}\right) dx\; dt \qquad (2.255)
\end{aligned}
$$

Since ΔJ_C does not depend on $(\Delta T_1)_C$ and $(\Delta T_2)_C$, the integrands containing $(\Delta T_1)_C$ or $(\Delta T_2)_C$ become zero. We thus have

$$
\begin{aligned}
&\frac{\partial}{\partial x}\left(K_1\frac{\partial \lambda_1}{\partial x}\right) + \frac{\partial (C\lambda_1)}{\partial t} + \sum_{i=2}^{M-1}(T_1 - Y_1)\delta(x - x_i) = 0 \\
&\frac{\partial}{\partial x}\left(K_2\frac{\partial \lambda_2}{\partial x}\right) + \frac{\partial (C\lambda_2)}{\partial t} + \sum_{i=2}^{M-1}(T_2 - Y_2)\delta(x - x_i) = 0 \\
&K_1\frac{\partial \lambda_1}{\partial x} - 2(T_1 - Y_1) = 0 \quad \text{at } x = 0 \\
&K_2\frac{\partial \lambda_2}{\partial x} - 2(T_2 - Y_2) = 0 \quad \text{at } x = 0 \\
&\lambda_1 = \lambda_2 = 0 \quad \text{at } x = 1 \\
&\lambda_1 = \lambda_2 = 0 \quad \text{at } t = t_f \qquad (2.256)
\end{aligned}
$$

Equation (2.255) now simplifies to

$$
\Delta J_C = -\int_{t=0}^{t_f}\int_{x=0}^{1}\Delta C\left(\lambda_1\frac{\partial T_1}{\partial t} + \lambda_2\frac{\partial T_2}{\partial t}\right) dx\; dt \qquad (2.257)
$$

From the definition ΔJ_C

$$
\Delta J_C = \int_{t=0}^{t_f}\int_{x=0}^{1} J'_C \Delta C\; dx\; dt \qquad (2.258)
$$

Comparing Equations (2.257) and (2.258) the following gradient equation is obtained:

$$J'_C = -\left(\lambda_1 \frac{\partial T_1}{\partial t} + \lambda_2 \frac{\partial T_2}{\partial t}\right) \tag{2.259}$$

The inverse technique for reconstructing $K_1(T_1, T_2)$, $K_2(T_1, T_2)$ and $C(T_1, T_2)$ can be cast in the following algorithmic form:

1. Assume the properties $K_1(x,t)$, $K_2(x,t)$ and $C(x,t)$; In the absence of additional information, they can be treated as constants.

2. Generate the corresponding state variables $T_1(x,t)$ and $T_2(x,t)$ by solving Equations (2.180-2.187).

3. Solve the adjoint problem, Equations (2.241-2.248), and obtain adjoint variables $\lambda_1(x)$ and $\lambda_2(x)$.

4. Compute J'_{K1}, J'_{K2} and J'_C from Equations (2.251), (2.252) and (2.259) respectively.

5. Calculate the conjugate coefficients ν_{K1}, ν_{K2} and ν_C form Equations (2.195), (2.196) and (2.197) respectively.

6. Estimate the directions of descent P_{K1}, P_{K2} and P_C from Equations (2.192), (2.193) and (2.194) respectively.

7. Solve the sensitivity problem, Equations (2.198- 2.215) to obtain sensitivity functions, $(\Delta T_1)_{K1}$, $(\Delta T_2)_{K1}$, $(\Delta T_1)_{K2}$, $(\Delta T_2)_{K2}$, $(\Delta T_1)_C$ and $(\Delta T_1)_C$.

8. Compute step sizes β_{K1}, β_{K2} and β_C using Equations (2.222-2.224).

9. Estimate K_1, K_2 and C using Equations (2.189-2.191).

10. Repeat the above calculation procedure until the discrepancy principle given by Equation (2.36) is satisfied.

2.5 Coupled Equations with Source Terms

The formulation of Section 2.4 is now extended to include source terms. The specific choice of the source terms is motivated by the study of multi-phase flow in porous media.

2.5.4 Sensitivity Analysis

Sensitivity Problem for K_1

$$\frac{\partial}{\partial x}\left[K_1\frac{\partial(\Delta T_1)_{K1}}{\partial x}\right]+\frac{\partial}{\partial x}\left[\Delta K_1\frac{\partial T_1}{\partial x}\right]=C\frac{\partial(\Delta T_1)_{K1}}{\partial t}-C\frac{\partial(\Delta T_2)_{K1}}{\partial t} \tag{2.268}$$

$$\frac{\partial}{\partial x}\left[K_2\frac{\partial(\Delta T_2)_{K1}}{\partial x}\right]=C\frac{\partial(\Delta T_2)_{K1}}{\partial t}-C\frac{\partial(\Delta T_1)_{K1}}{\partial t} \tag{2.269}$$

$$K_1\frac{\partial(\Delta T_1)_{K1}}{\partial x}+\Delta K_1\frac{\partial T_1}{\partial x}=0 \qquad \text{at} \quad x=0 \tag{2.270}$$

$$K_2\frac{\partial(\Delta T_2)_{K1}}{\partial x}=0 \qquad \text{at} \quad x=0 \tag{2.271}$$

$$(\Delta T_1)_{K1}=0 \qquad \text{and} \qquad (\Delta T_2)_{K1}=0 \qquad \text{at} \quad x=1 \tag{2.272}$$

$$(\Delta T_1)_{K1}=0 \qquad \text{and} \qquad (\Delta T_2)_{K1}=0 \qquad \text{at} \quad t=0 \tag{2.273}$$

Sensitivity Problem for K_2

$$\frac{\partial}{\partial x}\left[K_1\frac{\partial(\Delta T_1)_{K2}}{\partial x}\right]=C\frac{\partial(\Delta T_1)_{K2}}{\partial t}-C\frac{\partial(\Delta T_2)_{K2}}{\partial t} \tag{2.274}$$

$$\frac{\partial}{\partial x}\left[K_2\frac{\partial(\Delta T_2)_{K2}}{\partial x}\right]+\frac{\partial}{\partial x}\left[\Delta K_2\frac{\partial T_2}{\partial x}\right]=C\frac{\partial(\Delta T_2)_{K2}}{\partial t}-C\frac{\partial(\Delta T_1)_{K2}}{\partial t} \tag{2.275}$$

$$K_1\frac{\partial(\Delta T_1)_{K2}}{\partial x}=0 \qquad \text{at} \quad x=0 \tag{2.276}$$

$$K_2\frac{\partial(\Delta T_2)_{K2}}{\partial x}+\Delta K_2\frac{\partial T_2}{\partial x}=0 \qquad \text{at} \quad x=0 \tag{2.277}$$

$$(\Delta T_1)_{K2}=0 \qquad \text{and} \qquad (\Delta T_2)_{K2}=0 \qquad \text{at} \quad x=1 \tag{2.278}$$

$$(\Delta T_1)_{K2}=0 \qquad \text{and} \qquad (\Delta T_2)_{K2}=0 \qquad \text{at} \quad t=0 \tag{2.279}$$

Sensitivity Problem for C

$$\frac{\partial}{\partial x}\left[K_1\frac{\partial(\Delta T_1)_C}{\partial x}\right] = C\frac{\partial(\Delta T_1)_C}{\partial t} + \Delta C\frac{\partial T_1}{\partial t} - C\frac{\partial(\Delta T_2)_C}{\partial t} - \Delta C\frac{\partial T_2}{\partial t} \tag{2.280}$$

$$\frac{\partial}{\partial x}\left[K_2\frac{\partial(\Delta T_2)_C}{\partial x}\right] = C\frac{\partial(\Delta T_2)_C}{\partial t} + C\frac{\partial(\Delta T_2)_C}{\partial t} - C\frac{\partial(\Delta T_1)_C}{\partial t} - \Delta C\frac{\partial T_1}{\partial t} \tag{2.281}$$

$$K_1\frac{\partial(\Delta T_1)_C}{\partial x} = 0 \qquad \text{at} \quad x = 0 \tag{2.282}$$

$$K_2\frac{\partial(\Delta T_2)_C}{\partial x} = 0 \qquad \text{at} \quad x = 0 \tag{2.283}$$

$$(\Delta T_1)_C = 0 \qquad \text{and} \qquad (\Delta T_2)_C = 0 \qquad \text{at} \quad x = 1 \tag{2.284}$$

$$(\Delta T_1)_C = 0 \qquad \text{and} \qquad (\Delta T_2)_C = 0 \qquad \text{at} \quad t = 0 \tag{2.285}$$

2.5.5 Step Sizes

Equations (2.222-2.224) are applied to calculate step sizes, β_{K1}, β_{K2} and β_C.

2.5.6 Adjoint Problem and Gradient Equations

To derive the adjoint problem, Equation (2.260) is multiplied by the adjoint function, λ_1 and Equation (2.261) is multiplied by the adjoint function λ_2 and the resulting expression is integrated over the corresponding space and time domains. Then the result is added to the functional (2.188). We thus have the following expression of the functional:

$$\begin{aligned} J[K_1, K_2, C] &\equiv J[K_1(x,t), K_2(x,t), C(x,t)] = \\ &\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_1(x_i,t) - Y_1(x_i,t)]^2 dt + \int_{t=0}^{t_f}\sum_{i=1}^{M}[T_2(x_i,t) - Y_2(x_i,t)]^2 dt \\ &+ \int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_1\left[\frac{\partial}{\partial x}\left(K_1\frac{\partial T_1(x,t)}{\partial x}\right) - C\frac{\partial T_1(x,t)}{\partial t} + C\frac{\partial T_2(x,t)}{\partial t}\right] dx dt \\ &+ \int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_2\left[\frac{\partial}{\partial x}\left(K_2\frac{\partial T_2(x,t)}{\partial x}\right) - C\frac{\partial T_2(x,t)}{\partial t} + C\frac{\partial T_1(x,t)}{\partial t}\right] dx dt \end{aligned} \tag{2.286}$$

The variation ΔJ_{K1} is obtained by perturbing T_1 by $(\Delta T_1)_{K1}$ and T_2 by $(\Delta T_2)_{K2}$ in Equation (2.286). Then the original Equation (2.286) is subtracted from the resulting equation. After neglecting the higher-order terms we get the following expression of the variation ΔJ_{K1}:

$$\Delta J_{K1} =$$

$$2\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_1(x_i,t)-Y_1(x_i,t)](\Delta T_1)_{K1}dt + 2\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_2(x_i,t)-Y_2(x_i,t)](\Delta T_2)_{K1}dt$$
$$+\int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_1\left[\frac{\partial}{\partial x}\left(K_1\frac{\partial(\Delta T_1)_{K1}}{\partial x}\right)+\frac{\partial}{\partial x}\left(\Delta K_1\frac{\partial T_1}{\partial x}\right)-C\frac{\partial(\Delta T_1)_{K1}}{\partial t}+C\frac{\partial(\Delta T_2)_{K1}}{\partial t}\right]dxdt$$
$$+\int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_2\left[\frac{\partial}{\partial x}\left(K_2\frac{\partial(\Delta T_2)_{K1}}{\partial x}\right)-C\frac{\partial(\Delta T_2)_{K1}}{\partial t}+C\frac{\partial(\Delta T_1)_{K1}}{\partial t}\right]dxdt \qquad (2.287)$$

Or $\Delta J_{K1} =$

$$\int_{t=0}^{1}\left[\lambda_1 K_1\frac{\partial(\Delta T_1)_{K1}}{\partial x}\right]_{x=0}^{1}dt+\int_{t=0}^{t_f}\int_{x=0}^{1}(\Delta T_1)_{K1}\left[\frac{\partial}{\partial x}\left(K_1\frac{\partial\lambda_1}{\partial x}\right)\right]dxdt$$
$$-\int_{t=0}^{t_f}\left[(\Delta T_1)_{K1}K_1\frac{\partial\lambda_1}{\partial x}\right]_{x=0}^{1}dt+\int_{t=0}^{t_f}\left[\lambda_1\Delta K_1\frac{\partial T_1}{\partial x}\right]_{x=0}^{1}dt$$
$$-\int_{t=0}^{t_f}\int_{x=0}^{1}\Delta K_1\left[\frac{\partial\lambda_1}{\partial x}\frac{\partial T_1}{\partial x}\right]dxdt$$
$$-\int_{x=0}^{1}[C\lambda_1(\Delta T_1)_{K1}]_{t=0}^{t_f}dx+\int_{t=0}^{t_f}\int_{x=0}^{1}(\Delta T_1)_{K1}\frac{\partial(C\lambda_1)}{\partial t}dxdt$$
$$+\int_{x=0}^{1}[C\lambda_1(\Delta T_2)_{K1}]_{t=0}^{t_f}dx-\int_{t=0}^{t_f}\int_{x=0}^{1}(\Delta T_2)_{K1}\frac{\partial(C\lambda_1)}{\partial t}dxdt$$
$$+\int_{t=0}^{1}\left[\lambda_2 K_2\frac{\partial(\Delta T_2)_{K1}}{\partial x}\right]_{x=0}^{1}dt+\int_{t=0}^{t_f}\int_{x=0}^{1}(\Delta T_2)_{K1}\left[\frac{\partial}{\partial x}\left(K_2\frac{\partial\lambda_2}{\partial x}\right)\right]dxdt$$
$$-\int_{t=0}^{t_f}\left[(\Delta T_2)_{K1}K_2\frac{\partial\lambda_2}{\partial x}\right]_{x=0}^{1}dt-\int_{x=0}^{1}[C\lambda_2(\Delta T_2)_{K1}]_{t=0}^{t_f}dx$$
$$+\int_{t=0}^{t_f}\int_{x=0}^{1}(\Delta T_2)_{K1}\frac{\partial(C\lambda_2)}{\partial t}dxdt+\int_{x=0}^{1}[C\lambda_2(\Delta T_1)_{K1}]_{t=0}^{t_f}dx$$

$$
\begin{aligned}
&- \int_{t=0}^{t_f} \int_{x=0}^{1} (\Delta T_1)_{K1} \frac{\partial (C\lambda_2)}{\partial t} dx dt + 2 \int_{t=0}^{t_f} [(T_1 - Y_1)(\Delta T_1)_{K1}]_{x=0} \\
&+ 2 \int_{t=0}^{t_f} [(T_1 - Y_1)(\Delta T_1)_{K1}]_{x=1} + 2 \int_{t=0}^{t_f} \int_{x=0} \sum_{i=2}^{M} [T_1 - Y_1] \delta(x - x_i)(\Delta T_1)_{K1} dx dt \\
&+ 2 \int_{t=0}^{t_f} [(T_2 - Y_2)(\Delta T_2)_{K1}]_{x=0} + 2 \int_{t=0}^{t_f} [(T_2 - Y_2)(\Delta T_2)_{K1}]_{x=1} \\
&+ 2 \int_{t=0}^{t_f} \int_{x=0} \sum_{i=2}^{M} [T_2 - Y_2] \delta(x - x_i)(\Delta T_2)_{K1} dx dt
\end{aligned} \tag{2.288}
$$

Or $\Delta J_K =$

$$
\begin{aligned}
&\int_{t=0}^{t_f} \int_{x=0}^{1} (\Delta T_1)_{K1} \left[\frac{\partial}{\partial x} \left(K_1 \frac{\partial \lambda_1}{\partial x} \right) + \frac{\partial (C\lambda_1)}{\partial t} - \frac{\partial (C\lambda_2)}{\partial t} + 2 \sum_{i=2}^{M-1} [T_1 - Y_1] \delta(x - x_i) \right] dx dt \\
&+ \int_{t=0}^{t_f} (\Delta T_1)_{K1} \left[K_1 \frac{\partial \lambda_1}{\partial x} + 2(T_1 - Y_1) \right]_{x=0} dt - \int_{t=0}^{t_f} (\Delta T_1)_{K1} \left[K_1 \frac{\partial \lambda_1}{\partial x} - 2(T_1 - Y_1) \right]_{x=1} dt \\
&- \int_{x=0}^{1} [C\lambda_1 (\Delta T_1)_{K1}]_{t=0}^{t_f} dx + \int_{t=0}^{1} \lambda_1 \left[K_1 \frac{\partial (\Delta T_1)_{K1}}{\partial x} + \Delta K_1 \frac{\partial T_1}{\partial x} \right]_{x=0}^{1} dt \\
&+ \int_{t=0}^{t_f} \int_{x=0}^{1} (\Delta T_2)_{K1} \left[\frac{\partial}{\partial x} \left(K_2 \frac{\partial \lambda_2}{\partial x} \right) + \frac{\partial (C\lambda_2)}{\partial t} - \frac{\partial (C\lambda_1)}{\partial t} + 2 \sum_{i=2}^{M-1} [T_2 - Y_2] \delta(x - x_i) \right] dx dt \\
&+ \int_{t=0}^{t_f} (\Delta T_2)_{K1} \left[K2 \frac{\partial \lambda_2}{\partial x} + 2(T_2 - Y_2) \right]_{x=0} dt - \int_{t=0}^{t_f} (\Delta T_2)_{K1} \left[K_2 \frac{\partial \lambda_2}{\partial x} - 2(T_2 - Y_2) \right]_{x=1} dt \\
&- \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta K_1 \left[\frac{\partial \lambda_1}{\partial x} \frac{\partial T_1}{\partial x} \right] dx dt
\end{aligned} \tag{2.289}
$$

Now, the integrands containing $(\Delta T_1)_{K1}$ and $(\Delta T_2)_{K1}$ should be zero. Thus we have the following adjoint equations:

$$
\frac{\partial}{\partial x} \left(K_1 \frac{\partial \lambda_1}{\partial x} \right) + \frac{\partial (C\lambda_1)}{\partial t} - \frac{\partial (C\lambda_2)}{\partial t} + 2 \sum_{i=2}^{M-1} [T_1 - Y_1] \delta(x - x_i) = 0 \tag{2.290}
$$

$$
\frac{\partial}{\partial x} \left(K_2 \frac{\partial \lambda_2}{\partial x} \right) + \frac{\partial (C\lambda_2)}{\partial t} - \frac{\partial (C\lambda_1)}{\partial t} + 2 \sum_{i=2}^{M-1} [T_2 - Y_2] \delta(x - x_i) = 0 \tag{2.291}
$$

$$
K_1 \frac{\partial \lambda_1}{\partial x} + 2(T_1 - Y_1) = 0 \qquad \text{at} \quad x = 0 \tag{2.292}
$$

$$K_2\frac{\partial\lambda_2}{\partial x}+2(T_2-Y_2)=0 \qquad \text{at} \quad x=0 \tag{2.293}$$

$$\lambda_1=\lambda_2=0 \qquad \text{at} \quad x=1 \tag{2.294}$$

$$\lambda_1=\lambda_2=0 \qquad \text{for} \quad t=t_f \tag{2.295}$$

Equation (2.289) becomes

$$\Delta J_{K1}=-\int_{t=0}^{t_f}\int_{x=0}^{1}\Delta K_1\left[\frac{\partial\lambda_1}{\partial x}\frac{\partial T_1}{\partial x}\right]dxdt \tag{2.296}$$

From the definition of ΔJ_{K1} we have

$$\Delta J_{K1}=\int_{t=0}^{t_f}\int_{x=0}^{1}J'_{K1}(x,t)\Delta K_1\,dx\,dt \tag{2.297}$$

Comparing Equations (2.296) and (2.297) the following adjoint equation is obtained.

$$J'_{K1}=-\frac{\partial\lambda_1}{\partial x}\frac{\partial T_1}{\partial x} \tag{2.298}$$

The gradient of the functional with respect to K_2 is

$$J'_{K2}=-\frac{\partial\lambda_2}{\partial x}\frac{\partial T_2}{\partial x} \tag{2.299}$$

Let us derive the expression of J'_C. For deriving the expression for gradient of the functional with respect to C, we need to apply perturbation principle in Equation (2.286). It is assumed that when $C(x,t)$ undergoes a variation $\Delta C(x,t)$, $T_1(x,t)$ and $T_2(x,t)$ are perturbed by $T_1+(\Delta T_1)_C$ and $T_2+(\Delta T_2)_C$. Then replacing C by $C+\Delta C$, T_1 by $T_1+(\Delta T_1)_C$ and T_2 by $T_2+(\Delta T_2)_C$ in Equation (2.286), and subtracting from the resulting expressions Equation (2.286) and neglecting the higher-order terms, we get the variation of the functional as follows:

$$\begin{aligned}
\Delta J_C &= 2\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_1(x_i,t)-Y_1(x_i,t)](\Delta T_1)_C dt+2\int_{t=0}^{t_f}\sum_{i=1}^{M}[T_2(x_i,t)-Y_2(x_i,t)](\Delta T_2)_C dt\\
&+\int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_1\left[\frac{\partial}{\partial x}\left(K_1\frac{\partial(\Delta T_1)_C}{\partial x}\right)-\Delta C\frac{\partial T_1}{\partial t}-C\frac{\partial(\Delta T_1)_C}{\partial t}+\Delta C\frac{\partial T_2}{\partial t}+C\frac{\partial(\Delta T_2)_C}{\partial t}\right]dxdt\\
&+\int_{t=0}^{t_f}\int_{x=0}^{1}\lambda_2\left[\frac{\partial}{\partial x}\left(K_2\frac{\partial(\Delta T_2)_C}{\partial x}\right)-\Delta C\frac{\partial T_2}{\partial t}-C\frac{\partial(\Delta T_2)_C}{\partial t}+\Delta C\frac{\partial T_1}{\partial t}+C\frac{\partial(\Delta T_1)_C}{\partial t}\right]dxdt
\end{aligned}$$

Or $\Delta J_C =$

$$
\begin{aligned}
& 2\int_{t=0}^{t_f} [T_1(x_1,t) - Y_1(x_1,t)](\Delta T_1)_C dt + 2\int_{t=0}^{t_f} [T_2(x_1,t) - Y_2(x_1,t)](\Delta T_2)_C dt \\
+ \; & 2\int_{t=0}^{t_f} [T_1(x_M,t) - Y_1(x_M,t)](\Delta T_1)_C dt + 2\int_{t=0}^{t_f} [T_2(x_M,t) - Y_2(x_M,t)](\Delta T_2)_C dt \\
+ \; & 2\int_{t=0}^{t_f}\int_{x=0}^{1} \sum_{i=2}^{M-1} [T_1(x,t) - Y_1(x,t)](\Delta T_1)_C \delta(x - x_i) dx dt \\
+ \; & 2\int_{t=0}^{t_f}\int_{x=0}^{1} \sum_{i=2}^{M-1} [T_2(x,t) - Y_2(x,t)](\Delta T_2)_C \delta(x - x_i) dx dt \\
+ \; & \int_{t=0}^{t_f}\int_{x=0}^{1} \lambda_1 \left[\frac{\partial}{\partial x}\left(K_1 \frac{\partial(\Delta T_1)_C}{\partial x}\right) - C\frac{\partial(\Delta T_1)_C}{\partial t} + C\frac{\partial(\Delta T_2)_C}{\partial t}\right] dx dt \\
+ \; & \int_{t=0}^{t_f}\int_{x=0}^{1} \lambda_2 \left[\frac{\partial}{\partial x}\left(K_2 \frac{\partial(\Delta T_2)_C}{\partial x}\right) - C\frac{\partial(\Delta T_2)_C}{\partial t} + C\frac{\partial(\Delta T_1)_C}{\partial t}\right] dx dt \\
+ \; & \int_{t=0}^{t_f}\int_{x=0}^{1} \Delta C \left[(\lambda_1 - \lambda_2)\frac{\partial(T_2 - T_1)}{\partial t}\right] dx\, dt
\end{aligned}
\tag{2.300}
$$

Or $\Delta J_C =$

$$
\begin{aligned}
& \int_{t=0}^{t_f}\int_{x=0}^{1} (\Delta T_1)_C \left[\frac{\partial}{\partial x}\left(K_1 \frac{\partial \lambda_1}{\partial x}\right) + \frac{\partial(C\lambda_1)}{\partial t} - \frac{\partial(C\lambda_2)}{\partial t} + \sum_{i=2}^{M-1} (T_1 - Y_1)\delta(x - x_i)\right] dx dt \\
+ \; & \int_{t=0}^{t_f}\int_{x=0}^{1} (\Delta T_2)_C \left[\frac{\partial}{\partial x}\left(K_2 \frac{\partial \lambda_2}{\partial x}\right) + \frac{\partial(C\lambda_2)}{\partial t} - \frac{\partial(C\lambda_1)}{\partial t} + \sum_{i=2}^{M-1} (T_2 - Y_2)\delta(x - x_i)\right] dx dt \\
- \; & \int_{t=0}^{t_f} \left[(\Delta T_1)_C \left(K_1 \frac{\partial \lambda_1}{\partial x} - 2(T_1 - Y_1)\right)\right]_{x=0} dt \\
- \; & \int_{t=0}^{t_f} \left[(\Delta T_2)_C \left(K_2 \frac{\partial \lambda_2}{\partial x} - 2(T_2 - Y_2)\right)\right]_{x=0} dt \\
- \; & \int_{t=0}^{t_f} \left[\lambda_1 K_1 \frac{\partial(\Delta T_1)_C}{\partial x}\right]_{x=1} dt - \int_{t=0}^{t_f} \left[\lambda_2 K_2 \frac{\partial(\Delta T_2)_C}{\partial x}\right]_{x=1} dt \\
- \; & \int_{x=0}^{1} [\lambda_1 C(\Delta T_1)_C]_{t_f} dx - \int_{x=0}^{1} [\lambda_2 C(\Delta T_2)_C]_{t_f} dx
\end{aligned}
$$

$$+ \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta C \left[(\lambda_1 - \lambda_2) \frac{\partial (T_2 - T_1)}{\partial t} \right] dx \, dt \tag{2.301}$$

Since ΔJ_C does not depend $(\Delta T_1)_C$ and $(\Delta T_2)_C$, the integrands containing $(\Delta T_1)_C$ and $(\Delta T_2)_C$ are zero. Thus

$$\frac{\partial}{\partial x}\left(K_1 \frac{\partial \lambda_1}{\partial x}\right) + \frac{\partial (C\lambda_1)}{\partial t} - \frac{\partial (C\lambda_2)}{\partial t} + \sum_{i=2}^{M-1} (T_1 - Y_1)\delta(x - x_i) = 0 \tag{2.302}$$

$$\frac{\partial}{\partial x}\left(K_2 \frac{\partial \lambda_2}{\partial x}\right) + \frac{\partial (C\lambda_2)}{\partial t} - \frac{\partial (C\lambda_1)}{\partial t} + \sum_{i=2}^{M-1} (T_2 - Y_2)\delta(x - x_i) = 0 \tag{2.303}$$

$$K_1 \frac{\partial \lambda_1}{\partial x} - 2(T_1 - Y_1) = 0 \quad \text{at } x = 0 \tag{2.304}$$

$$K_2 \frac{\partial \lambda_2}{\partial x} - 2(T_2 - Y_2) = 0 \quad \text{at } x = 0 \tag{2.305}$$

$$\lambda_1 = \lambda_2 = 0 \quad \text{at } x = 1 \tag{2.306}$$

$$\lambda_1 = \lambda_2 = 0 \quad \text{for } t = t_f \tag{2.307}$$

Equation (2.301) now simplifies to

$$\Delta J_C = \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta C \left[(\lambda_1 - \lambda_2) \frac{\partial (T_2 - T_1)}{\partial t} \right] dx \, dt \tag{2.308}$$

From the definition of ΔJ_C

$$\Delta J_C = \int_{t=0}^{t_f} \int_{x=0}^{1} \Delta C J'_C(x,t) \, dx \, dt \tag{2.309}$$

Comparing Equations (2.308) and (2.309) we have

$$J'_C = (\lambda_1 - \lambda_2) \frac{\partial (T_2 - T_1)}{\partial t} \tag{2.310}$$

The inverse technique for reconstructing $K_1(T_1, T_2)$, $K_2(T_1, T_2)$ and $C(T_1, T_2)$ can be cast in the following algorithmic form:

1. Assume the properties $K_1(x,t)$, $K_2(x,t)$ and $C(x,t)$; In the absence of additional information, they can be treated as constants.

2. Generate the corresponding state variables $T_1(x,t)$ and $T_2(x,t)$ by solving Equations (2.260-2.267).

3. Solve the adjoint problem, Equations (2.302-2.307), and obtain adjoint variables $\lambda_1(x)$ and $\lambda_2(x)$.

4. Compute J'_{K1}, J'_{K2} and J'_C from Equations (2.298), (2.299) and (2.310) respectively.

5. Calculate the conjugate coefficients ν_{K1}, ν_{K2} and ν_C form Equations (2.195), (2.196) and (2.197) respectively.

6. Estimate the directions of descent P_{K1}, P_{K2} and P_C from Equations (2.192), (2.193) and (2.194) respectively.

7. Solve the sensitivity problem, Equations (2.268- 2.285) to obtain sensitivity functions, $(\Delta T_1)_{K1}$, $(\Delta T_2)_{K1}$, $(\Delta T_1)_{K2}$, $(\Delta T_2)_{K2}$, $(\Delta T_1)_C$ and $(\Delta T_1)_C$.

8. Compute step sizes β_{K1}, β_{K2} and β_C using Equations (2.222-2.224).

9. Estimate K_1, K_2 and C using Equations (2.189-2.191).

10. Repeat the above calculation procedure until the discrepancy principle given by Equation (2.36) is satisfied.

2.6 Determination of Constitutive Relationships for Oil-Water Flow

One of the applications of coupled inverse procedure to a practical problem is demonstrated in this section. For a flow of two homogeneous immiscible incompressible fluids, oil and water for example in an isotropic porous medium, the continuity equations are given by [*Bear(1972)*]

$$\epsilon\frac{\partial S_w}{\partial \bar{t}} - \frac{\partial}{\partial \bar{x}}\left[\left(\frac{KK_{rw}(S_w, S_o)}{\nu_w}\right)\frac{\partial \bar{P}_w}{\partial \bar{x}}\right] = 0 \tag{2.311}$$

$$\epsilon\frac{\partial S_o}{\partial \bar{t}} - \frac{\partial}{\partial \bar{x}}\left[\left(\frac{KK_{ro}(S_w, S_o)}{\nu_o}\right)\frac{\partial \bar{P}_o}{\partial \bar{x}}\right] = 0 \tag{2.312}$$

With the following initial and boundary conditions:

$$\bar{P}_w = \bar{P}_{wi} \quad \text{for} \quad \bar{t} = 0 \tag{2.313}$$

$$\bar{P}_o = \bar{P}_{oi} \quad \text{at} \quad \bar{t} = 0 \tag{2.314}$$

$$-\frac{KK_{rw}}{\nu_w}\frac{\partial \bar{P}_w}{\partial \bar{x}} = \bar{q}_w \quad \text{at} \quad \bar{x} = 0 \tag{2.315}$$

$$-\frac{KK_{ro}}{\nu_w}\frac{\partial \bar{P}_o}{\partial \bar{x}} = \bar{q}_o \quad \text{at} \quad \bar{x} = 0 \tag{2.316}$$

$$\bar{P}_w = \bar{P}_{w1} \quad \text{at} \quad \bar{x} = \bar{L} \tag{2.317}$$

$$\bar{P}_o = \bar{P}_{o1} \quad \text{at} \quad \bar{x} = \bar{L} \tag{2.318}$$

where the parameters K_{rw} and K_{ro} are functions of water and oil saturations S_w and S_o. Since there are only two fluids in the medium, the sum of S_w and S_o is unity. Hence K_{rw} and K_{ro} are effectively functions of S_w. Now we define capillary pressure by

$$\bar{P}_c = \bar{P}_o - \bar{P}_w$$

Provided near-equilibrium conditions prevail, the capillary pressure, $\bar{P}_c$ is only a function of S_w. Let water saturation, S_w be expressed as

$$S_w = f(\bar{P}_c) = f(\bar{P}_O - \bar{P}_w)$$

Equation (2.311) can be written as

$$\epsilon\frac{\partial f(\bar{P}_c)}{\partial \bar{t}} - \frac{\partial}{\partial \bar{x}}\left[\left(\frac{KK_{rw}(\bar{P}_c)}{\bar{\nu}_w}\right)\frac{\partial \bar{P}_w}{\partial \bar{x}}\right] = 0$$

$$\text{Or} \quad \epsilon\frac{df}{d\bar{P}_c}\frac{\partial \bar{P}_c}{\partial \bar{t}} - \frac{\partial}{\partial \bar{x}}\left[\left(\frac{KK_{rw}(\bar{P}_c)}{\bar{\nu}_w}\right)\frac{\partial \bar{P}_w}{\partial \bar{x}}\right] = 0$$

$$\text{Or} \quad \left(\epsilon\frac{df}{d\bar{P}_c}\right)\left(\frac{\partial \bar{P}_o}{\partial \bar{t}} - \frac{\partial \bar{P}_w}{\partial \bar{t}}\right) - \frac{\partial}{\partial \bar{x}}\left[\left(\frac{KK_{rw}(\bar{P}_c)}{\bar{\nu}_w}\right)\frac{\partial \bar{P}_w}{\partial \bar{x}}\right] = 0$$

$$\text{Or} \quad \frac{\partial}{\partial \bar{x}}\left[\left(\frac{KK_{rw}(\bar{P}_c)}{\bar{\nu}_w}\right)\frac{\partial \bar{P}_w}{\partial \bar{x}}\right] - \bar{C}\frac{\partial \bar{P}_w}{\partial \bar{t}} = -\bar{C}\frac{\partial \bar{P}_o}{\partial \bar{t}} \tag{2.319}$$

where the notation

$$\bar{C} = -\epsilon\frac{df}{d\bar{P}_c} \tag{2.320}$$

has been used. Since $S_w = 1 - S_o$, Equation (2.312) can be written as

$$\epsilon\frac{\partial S_w}{\partial \bar{t}} - \frac{\partial}{\partial \bar{x}}\left[\left(\frac{KK_{ro}(\bar{P}_c)}{\bar{\nu}_o}\right)\frac{\partial \bar{P}_o}{\partial \bar{x}}\right] = 0$$

$$\text{Or} \quad \frac{\partial}{\partial \bar{x}}\left[\left(\frac{KK_{ro}(\bar{P}_c)}{\bar{\nu}_o}\right)\frac{\partial \bar{P}_o}{\partial \bar{x}}\right] - \bar{C}\frac{\partial \bar{P}_o}{\partial \bar{t}} = -\bar{C}\frac{\partial \bar{P}_w}{\partial \bar{t}} \tag{2.321}$$

With the following dimensionless quantities

$$x = \frac{\bar{x}}{\bar{L}}, \quad P_w = \frac{\bar{P}_w}{\bar{P}_r}, \quad P_o = \frac{\bar{P}_o}{\bar{P}_r}, \quad P_c = \frac{\bar{P}_c}{\bar{P}_r},$$
$$t = \frac{\bar{t}\bar{K}P_r}{\bar{\nu}_r L^2}, \quad C = \epsilon\frac{df}{dP_c}, \quad K_w = \frac{K_{rw}\bar{\nu}_r}{\bar{\nu}_w}, \quad K_o = \frac{K_{ro}\bar{\nu}_r}{\bar{\nu}_o} \tag{2.322}$$

we get dimensionless form of Equations (2.311-2.318) as follows:

$$\frac{\partial}{\partial x}\left(K_w\frac{\partial P_w}{\partial x}\right) - C\frac{\partial P_w}{\partial t} = -C\frac{\partial P_o}{\partial t} \tag{2.323}$$

$$\frac{\partial}{\partial x}\left(K_o\frac{\partial P_o}{\partial x}\right) - C\frac{\partial P_o}{\partial t} = -C\frac{\partial P_w}{\partial t} \tag{2.324}$$

$$P_w = P_{wi} \quad \text{for} \quad t = 0 \tag{2.325}$$

$$P_o = P_{oi} \quad \text{for} \quad t = 0 \tag{2.326}$$

$$-K_w\frac{\partial P_w}{\partial x} = q_w \quad \text{at} \quad x = 0 \tag{2.327}$$

$$-K_o\frac{\partial P_o}{\partial x} = q_o \quad \text{at} \quad x = 0 \tag{2.328}$$

$$P_w = P_{wl} \quad \text{at} \quad x = 1 \tag{2.329}$$

$$P_o = P_{ol} \quad \text{at} \quad x = 1 \tag{2.330}$$

Equations (2.323-2.330) are similar to Equations (2.260-2.267). Therefore the sensitivity Equations and adjoint equations are similar to the sensitivity Equations (2.268-2.285) and adjoint Equations (2.302-2.307) respectively derived in Section 2.5. These are repeated below for completeness.

2.6.1 Sensitivity Problem

Sensitivity Problem for K_w

$$\frac{\partial}{\partial x}\left(K_w\frac{\partial(\Delta P_w)_{Kw}}{\partial x}\right) + \frac{\partial}{\partial x}\left(\Delta K_w\frac{\partial P_w}{\partial x}\right) - C\frac{\partial(\Delta P_w)_{Kw}}{\partial t} = -C\frac{\partial(\Delta P_o)_{Kw}}{\partial t} \tag{2.331}$$

$$\frac{\partial}{\partial x}\left(K_o\frac{\partial(\Delta P_o)_{Kw}}{\partial x}\right) - C\frac{\partial(\Delta P_o)_{Kw}}{\partial t} = -C\frac{\partial(\Delta P_w)}{\partial t} \tag{2.332}$$

$$-K_w\frac{\partial(\Delta P_w)_{Kw}}{\partial x} - \Delta K_w\frac{\partial P_w}{\partial x} = 0 \quad \text{at} \quad x = 0 \tag{2.333}$$

$$-K_o\frac{\partial(\Delta P_o)_{Kw}}{\partial x} = 0 \quad \text{at} \quad x = 0 \tag{2.334}$$

$$(\Delta P_w)_{Kw} = (\Delta P_o)_{Kw} = 0 \quad \text{at} \quad x = 1 \tag{2.335}$$

$$(\Delta P_w)_{Kw} = (\Delta P_o)_{Kw} = 0 \quad \text{for} \quad t = 0 \tag{2.336}$$

Sensitivity Problem for K_o

$$\frac{\partial}{\partial x}\left(K_w\frac{\partial(\Delta P_w)_{Ko}}{\partial x}\right) - C\frac{\partial(\Delta P_w)_{Ko}}{\partial t} = -C\frac{\partial(\Delta P_o)}{\partial t} \tag{2.337}$$

$$\frac{\partial}{\partial x}\left(K_o\frac{\partial(\Delta P_o)_{Ko}}{\partial x}\right) + \frac{\partial}{\partial x}\left(\Delta K_o\frac{\partial P_o}{\partial x}\right) - C\frac{\partial(\Delta P_o)_{Ko}}{\partial t} = -C\frac{\partial(\Delta P_w)_{Ko}}{\partial t} \tag{2.338}$$

$$-K_w\frac{\partial(\Delta P_w)_{Ko}}{\partial x} = 0 \quad \text{at} \quad x = 0 \tag{2.339}$$

$$-K_o\frac{\partial(\Delta P_o)_{Ko}}{\partial x} - \Delta K_o\frac{\partial P_o}{\partial x} = 0 \quad \text{at} \quad x = 0 \tag{2.340}$$

$$(\Delta P_w)_{Ko} = (\Delta P_o)_{Ko} = 0 \quad \text{at} \quad x = 1 \tag{2.341}$$

$$(\Delta P_w)_{Ko} = (\Delta P_o)_{Ko} = 0 \quad \text{for} \quad t = 0 \tag{2.342}$$

Sensitivity Problem for C

$$\frac{\partial}{\partial x}\left(K_w\frac{\partial(\Delta P_w)_C}{\partial x}\right)-C\frac{\partial(\Delta P_w)_C}{\partial t}-\Delta C\frac{\partial P_w}{\partial t}=-C\frac{\partial(\Delta P_o)}{\partial t}-\Delta C\frac{\partial P_o}{\partial t} \quad (2.343)$$

$$\frac{\partial}{\partial x}\left(K_o\frac{\partial(\Delta P_o)_C}{\partial x}\right)-C\frac{\partial(\Delta P_o)_C}{\partial t}-\Delta C\frac{\partial P_o}{\partial t}=-C\frac{\partial(\Delta P_w)_C}{\partial t}-\Delta C\frac{\partial P_w}{\partial t} \quad (2.344)$$

$$-K_w\frac{\partial(\Delta P_w)_C}{\partial x}=0 \quad \text{at} \quad x=0 \quad (2.345)$$

$$-K_o\frac{\partial(\Delta P_o)_C}{\partial x}=0 \quad \text{at} \quad x=0 \quad (2.346)$$

$$(\Delta P_w)_C=(\Delta P_o)_C=0 \quad \text{at} \quad x=1 \quad (2.347)$$

$$(\Delta P_w)_C=(\Delta P_o)_C=0 \quad \text{for} \quad t=0 \quad (2.348)$$

Adjoint Problem

$$\frac{\partial}{\partial x}\left(K_1\frac{\partial\lambda_1}{\partial x}\right)+\frac{\partial(C\lambda_1)}{\partial t}-\frac{\partial(C\lambda_2)}{\partial t}+2\sum_{i=2}^{M-1}[P_w-P_{we}]\delta(x-x_i)=0 \quad (2.349)$$

$$\frac{\partial}{\partial x}\left(K_2\frac{\partial\lambda_2}{\partial x}\right)+\frac{\partial(C\lambda_2)}{\partial t}-\frac{\partial(C\lambda_1)}{\partial t}+2\sum_{i=2}^{M-1}[P_o-P_{oe}]\delta(x-x_i)=0 \quad (2.350)$$

$$K_1\frac{\partial\lambda_1}{\partial x}+2(P_w-P_{we})=0 \quad \text{at} \quad x=0 \quad (2.351)$$

$$K_2\frac{\partial\lambda_2}{\partial x}+2(P_o-P_{oe})=0 \quad \text{at} \quad x=0 \quad (2.352)$$

$$\lambda_1=\lambda_2=0 \quad \text{at} \quad x=1 \quad (2.353)$$

$$\lambda_1=\lambda_2=0 \quad \text{for} \quad t=t_f \quad (2.354)$$

Gradient Equations

$$J'_{Kw} = -\frac{\partial P_w}{\partial x}\frac{\partial \lambda_1}{\partial x} \quad (2.355)$$

$$J'_{Ko} = -\frac{\partial P_o}{\partial x}\frac{\partial \lambda_2}{\partial x} \quad (2.356)$$

$$J'_{C} = (\lambda_2 - \lambda_1)\left(\frac{\partial P_w}{\partial t} - \frac{\partial P_o}{\partial t}\right) \quad (2.357)$$

2.7 Generalization to Multi-dimensional cases

The inverse problem discussed in the earlier sections was restricted to one spatial dimension. The generalization of this theory is taken up next. The governing equations of physical processes can be represented as:

$$L(u, p; x, t) = 0 \quad (2.358)$$

where

$$u = (u_1, u_2 \cdots u_N)^T \quad (2.359)$$

$$p = (p_1, p_2 \cdots p_M)^T \quad (2.360)$$

$$L = (L_1, L_2 \cdots L_N)^T \quad (2.361)$$

x represents the spatial coordinates and t is time. The initial conditions are

$$u = f_0 \quad \text{when} \quad t = t_0 \quad (2.362)$$

and the boundary conditions are

$$L_{UB} = f_1 \quad \text{on} \quad (\Gamma_{UB}) \quad (2.363)$$

$$L_{LB} = f_2 \quad \text{on} \quad (\Gamma_{LB}) \quad (2.364)$$

where L_{UB} and L_{LB} are vector operators representing boundary conditions, $(u_1, u_2, \cdots u_N)$ are N state variables and $(p_1, p_2, \cdots p_M)$ are M parameters. In the direct problem, we need to find the unknown state u when parameter p and all initial and boundary conditions are known. In contrast to the direct problem, the inverse problem seeks to find the unknown

parameters p (it may also include the unknown initial or boundary conditions) when continuous or discrete observations of state u are given. This can be stated as

$$\begin{aligned} &\text{find } p \in Ad \\ &\text{such that } \; u(p) = z \quad at\ Ob \end{aligned} \tag{2.365}$$

where Ad is an admissible set of unknown parameters, and Ob is the observation set of space and time where the records of states z are taken.

Because of measurement and model errors, problem (2.358) has no exact solution. The problem has to be solved approximately by an optimization procedure. This is equivalent to

$$\begin{aligned} &\text{to find} p \in Ad \\ &\text{such that} J(p) = \min_{p \in Ad} J(p) \end{aligned} \tag{2.366}$$

where

$$J(p) = \int_{t=0}^{t_f} \int_{\Gamma_{LB}}^{\Gamma_{UB}} [u_i(p) - z_i)]^2 \, d\Omega \, dt \tag{2.367}$$

where vector $[u_i(p) - z_i]$ represents the difference between the model output of u_i and its observations set Ob.

2.7.1 Inverse Solution Methods

Numerical solution of the optimization problem (2.366) can be classified into the following three categories:

- Gauss-Newton
- Gradient Search
- Direct Search

In order to obtain the Gauss-Newton direction it is necessary to calculate the following sensitivity matrix in each iteration of the non-linear least squares minimization:

$$J_w = \begin{pmatrix} \frac{\partial u_1}{\partial p_1} & \frac{\partial u_2}{\partial p_1} & \cdots \frac{\partial u_N}{\partial p_1} \\ \frac{\partial u_1}{\partial p_2} & \frac{\partial u_2}{\partial p_2} & \cdots \frac{\partial u_N}{\partial p_2} \\ \cdots & \cdots & \cdots \\ \frac{\partial u_1}{\partial p_M} & \frac{\partial u_2}{\partial p_M} & \cdots \frac{\partial u_N}{\partial p_M} \end{pmatrix} \tag{2.368}$$

where $[\frac{\partial u_i}{\partial p_j}]$ is the sensitivity matrix of the discretized state u_i with respect to the discretized unknown parameter p_j. Gradient search methods are used to avoid the calculation of the sensitivity matrix. Hence less computer time is required. Direct search methods do not require the calculation of sensitivity matrix (2.368) or the gradient vector but the rate of convergence of such methods is generally slow. The grad search method is presented in the sections below.

2.7.2 Direct Problem

It is clear that the unknown quantities $u_1, u_2 \cdots u_N$ in Equations (2.358-2.364) are assumed to be known while $p_1, p_2, \cdots p_M$ are known. While generating simulated state variables $u_1, u_2, \cdots u_N$, i.e. $p_1, p_2, \cdots p_M$ to calculate $u_1, u_2, \cdots u_N$ the direct problem (2.358-2.364) is nonlinear since the parameters $p_1, p_2, \cdots p_M$ are functions of $u_1, u_2, \cdots u_N$. Therefore an iterative technique is needed for solving the problem a with finite difference method.

2.7.3 Conjugate Gradient Method For Minimization

The following iterative process based on the conjugate gradient method is used for estimation of $p_1, p_2 \cdots p_M$ by minimizing the functional $J(p)$.

$$\hat{p}_i^{n+1}(x,t) = \hat{p}_i^n(x,t) - \beta_i^n P_i^n(x,t) \tag{2.369}$$

for $n = 0, 1, 2, \cdots$ and $i = 1, 2, \cdots M$ where β_i^n is step sizes for $\hat{p}_i$ in going from iteration n to $(n+1)$ and P_i^n is the direction of descent for $\hat{p}_i$. The directions of descent are given by

$$P_i^n(x,t) = J_i'^n + \nu_i^n P_i^{n-1}(x,t) \tag{2.370}$$

which is the conjugation of the gradient direction J'^{n}_{i} at the iteration n and the direction of descent $P^{n-1}_{i}(x,t)$ at iteration $(n-1)$. The conjugation coefficient ν^{n}_{i} is given by

$$\nu^{n}_{i} = \frac{\int_{\Gamma_1}^{\Gamma_2}\int_{t_0}^{t_f}(J'^{n}_{i})^2 dt dx}{\int_{\Gamma_1}^{\Gamma_2}\int_{t_0}^{t_f}(J'^{n-1}_{i})^2 dt dx} \tag{2.371}$$

To perform the iteration according to Equation (2.369), we need to compute the step sizes $\beta^{n}_{1}, \beta^{n}_{2}, \cdots \beta^{n}_{m}$ and the gradient of the functional $J'^{n}_{1}, J'^{n}_{2}, \cdots J'^{n}_{M}$. In order to determine these quantities, the 'sensitivity problem' and 'adjoint problem' are constructed as follows.

2.7.4 Sensitivity Analysis

In order to derive the sensitivity problem for each unknown parameter, we should perturb the unknown parameters one at a time. Applying perturbation principle in the Equations (2.358,2.362,2.363 and 2.364) the following sensitivity problems are obtained.

$$\nabla_u L \delta u + \nabla_p L \delta p = 0 \tag{2.372}$$

$$\delta u = 0 \quad when \quad t = t_0 \tag{2.373}$$

$$\nabla_u L_{UB} \delta u + \nabla_p L_{UB} \delta p = 0 \quad on \quad \Gamma_{UB} \tag{2.374}$$

$$\nabla_u L_{LB} \delta u + \nabla_p L_{LB} \delta p = 0 \quad on \quad \Gamma_{LB} \tag{2.375}$$

where $\nabla_u L$ and $\nabla_p L$ are the gradient operators of L with respect to u and p respectively. These are given by

$$\nabla_u L = \begin{pmatrix} \frac{\partial L_1}{\partial u_1} & \frac{\partial L_1}{\partial u_2} & \cdots \frac{\partial L_1}{\partial u_N} \\ \frac{\partial L_2}{\partial u_1} & \frac{\partial L_2}{\partial u_2} & \cdots \frac{\partial L_2}{\partial u_N} \\ \cdots & \cdots & \cdots \\ \frac{\partial L_N}{\partial u_1} & \frac{\partial L_N}{\partial u_2} & \cdots \frac{\partial L_N}{\partial u_N} \end{pmatrix} \tag{2.376}$$

$$\nabla_p L = \begin{pmatrix} \frac{\partial L_1}{\partial p_1} & \frac{\partial L_1}{\partial p_2} & \cdots \frac{\partial L_1}{\partial p_M} \\ \frac{\partial L_2}{\partial p_1} & \frac{\partial L_2}{\partial p_2} & \cdots \frac{\partial L_2}{\partial p_M} \\ \cdots & \cdots & \cdots \\ \frac{\partial L_N}{\partial p_1} & \frac{\partial L_N}{\partial p_2} & \cdots \frac{\partial L_N}{\partial p_M} \end{pmatrix} \tag{2.377}$$

when $\nabla_u L_{UB}$, $\nabla_p L_{UB}$, $\nabla_u L_{LB}$ and $\nabla_p L_{LB}$ have the same meaning as above.
δu is given by the matrix $[\Delta u_{i,j}]$ where $\Delta u_{i,j}$ denotes the change in u_i due to change in

the parameter p_j. The change in parameter p_j is given by Δp_j. Again δp is given by the vector

$$\delta p = [\Delta p_1, \Delta p_2, \cdots \Delta p_M]^T$$

For the above sensitivity problem we need to change only one parameter at a time. Let us consider the effect of change in one parameter p_k. In that case all the elements except Δp_k will be zero. For the matrix δu we have

$$\begin{aligned} \Delta u_{i,j} &= 0 \qquad \text{if} \quad j \neq k \\ \Delta u_{i,j} &= \Delta u_{i,k} \qquad \text{if} \quad j = k \end{aligned}$$

The adjoint form of matrices $\nabla_u L$ and $\nabla_p L$ are given by

$$\nabla_u^* L = \begin{pmatrix} \left(\frac{\partial L_1}{\partial u_1}\right)^* & \left(\frac{\partial L_1}{\partial u_2}\right)^* & \cdots \left(\frac{\partial L_1}{\partial u_N}\right)^* \\ \left(\frac{\partial L_2}{\partial u_1}\right)^* & \left(\frac{\partial L_2}{\partial u_2}\right)^* & \cdots \left(\frac{\partial L_2}{\partial u_N}\right)^* \\ \cdots & \cdots & \cdots \\ \left(\frac{\partial L_N}{\partial u_1}\right)^* & \left(\frac{\partial L_N}{\partial u_2}\right)^* & \cdots \left(\frac{\partial L_N}{\partial u_N}\right)^* \end{pmatrix} \tag{2.378}$$

$$\nabla_p^* L = \begin{pmatrix} \left(\frac{\partial L_1}{\partial p_1}\right)^* & \left(\frac{\partial L_1}{\partial p_2}\right)^* & \cdots \left(\frac{\partial L_1}{\partial p_M}\right)^* \\ \left(\frac{\partial L_2}{\partial p_1}\right)^* & \left(\frac{\partial L_2}{\partial p_2}\right)^* & \cdots \left(\frac{\partial L_2}{\partial p_M}\right)^* \\ \cdots & \cdots & \cdots \\ \left(\frac{\partial L_N}{\partial p_1}\right)^* & \left(\frac{\partial L_N}{\partial p_2}\right)^* & \cdots \left(\frac{\partial L_N}{\partial p_M}\right)^* \end{pmatrix} \tag{2.379}$$

The transpose of the matrices ∇_u^* and ∇_p^* are denoted respectively by ∇_u^+ and ∇_p^+ The function to be minimized is given by

$$J(p) = \int_{t=t_0}^{t_f} \int_{\Omega} f[u(p)] d\Omega dt \tag{2.380}$$

where $f[u(p)]$ is a user-chosen function.[The choice $(T(x) - Y_i)^2$ is one of the many possible for the function f.] The functional $J(\hat{p})$ for iteration $(n+1)$ is obtained as

$$J(\hat{p}^{n+1}) = \int_{t=t_0}^{t_f} \int_{\Omega} f[u(\hat{p}^n - \beta^n P^n)] d\Omega dt \tag{2.381}$$

Applying Taylor series expansion and neglecting second and higher order terms we get,

$$\begin{aligned} u(\hat{p}^n - \beta^n P^n) &= u(\hat{p}^n) - \beta^n P^n \frac{\partial u}{\partial p} \\ &= u(\hat{p}^n) - \beta^n \delta u^n \end{aligned} \tag{2.382}$$

Hence we have

$$J(\hat{p}^{n+1}) = \int_{t_0}^{t_f}\int_{\Omega} f[u(\hat{p}^n) - \beta^n \delta u^n] d\Omega dt$$
$$= \int_{t=t_0}^{t_f}\int_{\Omega} \left[f[u(\hat{p}^n)] - \beta^n \delta u^n \frac{\partial f}{\partial u} \cdots \right] d\Omega dt \tag{2.383}$$

Now, we have to determine β^n in such a way that J^{n+1} is minimum. Hence,

$$\frac{\partial J^{n+1}}{\partial \beta^n} = 0 \tag{2.384}$$

This will produce M equations for $\beta_1^n, \beta_2^n, \cdots \beta_M^n$. The quantities δu^n are calculated from Equations (2.372-2.375) and P^n is estimated from Equations (2.370). From Equations (2.370 and 2.371) it is clear that P^n is known when the gradient direction J'^n is known. These gradient directions are calculated from the following adjoint problem.

2.7.5 Adjoint Problem and Gradient Equations

We need to find p such that $J(p)$ will be optimized and Equations (2.358-2.364) are satisfied. Hence the functional $J(p)$ can be written as,

$$J(p) = \int_{t=t_0}^{t_f}\int_{\Omega} f(p) d\Omega dt + \int_{t=t_0}^{t_f}\int_{\Omega} \lambda L(u,p) d\Omega dt \tag{2.385}$$

where $\lambda = [\lambda_1, \lambda_2, \cdots \lambda_N]^T$ are the adjoint functions for the N equations. If $N = 1$, i.e. for one equation model, example heat conduction problem, there is only one adjoint function (λ_1).

For a two equations model like oil-water flow through porous media, there are two adjoint functions (λ_1 and λ_2)
The variation of the objective function (2.367) δJ is obtained by perturbing u by δu in Equation (2.367), subtracting from the resulting expression the original Equation (2.367) and neglecting the higher order terms. We thus obtain

$$\delta J = \int_{t=t_0}^{t_f}\int_{\Omega} \left[\frac{\partial f}{\partial u}\delta u + \frac{\partial f}{\partial p}\delta p \right] d\Omega dt + \int_{t=t_0}^{t_f}\int_{\Omega} \lambda \left[\nabla_u L \delta u + \nabla_p L \delta p \right] d\Omega dt \tag{2.386}$$

We define the scalar product of any two vector functions u and v on Ω and the time interval $[t_0, t_f]$ as

$$(u,v)_{\Omega,T} = \int_{t=t_0}^{t_f} \int_{\Omega} (uv)\, d\Omega dt \tag{2.387}$$

At the boundaries the above product is defined by

$$(u,v)_{\Gamma_{UB},T} = \int_{t=t_0}^{t_f} (uv)|_{\Gamma_{UB}} dt \tag{2.388}$$

$$(u,v)_{\Gamma_{LB},T} = \int_{t=t_0}^{t_f} (uv)|_{\Gamma_{LB}} dt \tag{2.389}$$

Using Green's formula several times to transfer the differential operator from δu or δp to λ we obtain

$$\int_{t=t_0}^{t_f} \int_{\Omega} \lambda(\nabla_u L \delta u) d\Omega dt = (\lambda, \nabla_u L \delta u)_{\Omega,T} = (\delta u, \nabla_u^+ L \lambda)_{\Omega,T} + BIT \tag{2.390}$$

$$\int_{t=t_0}^{t_f} \int_{\Omega} \lambda(\nabla_p L \delta p) d\Omega dt = (\lambda, \nabla_p L \delta p)_{\Omega,T} = (\delta p, \nabla_u^+ L \lambda)_{\Omega,T} + BIT \tag{2.391}$$

where BIT denotes all boundary integral terms and $\nabla_u^+ L$ and $\nabla_p^+ L$ are transposed adjoint operators of $\nabla_u L$ and $\nabla_p L$ respectively. From equations (2.386,2.390 and 2.391) we get the following expression for δJ:

$$\delta J = \left(\delta u, \nabla_u^+ L\lambda + \frac{\partial f}{\partial u}\right)_{\Omega,T} + \left(\delta p, \nabla_p^+ L\lambda + \frac{\partial f}{\partial p}\right)_{\Omega,T} + BIT \tag{2.392}$$

where the term BIT in (2.392) is expressed as

$$\begin{aligned} BIT &= (\delta p, \nabla_p^+ L_{UB}\lambda)_{\Gamma_{UB},T} - (\delta p, \nabla_p^+ L_{LB}\lambda)_{\Gamma_{LB},T} + (\delta u, \nabla_u^+ L_{UB}\lambda)_{\Gamma_{UB},T} \\ &- (\delta u, \nabla_u^+ L_{LB}\lambda)_{\Gamma_{LB},T} + (\delta u \frac{\partial f}{\partial u})_{\Gamma_{UB},T} + (\delta u \frac{\partial f}{\partial u})_{\Gamma_{LB},T} + (\delta u, \lambda)_{\Omega,t_f} - (\lambda, \delta u)_{\Omega,t_0} \\ &- (\lambda, \nabla_u L_{UB}\delta u + \nabla_p L_{UB}\delta p)_{\Gamma_{UB},T} - (\lambda, \nabla_u L_{LB}\delta u + \nabla_p L_{LB}\delta p)_{\Gamma_{LB},T} \end{aligned} \tag{2.393}$$

From Equations (2.375-2.375) it is clear that the last three terms of the expression of BIT are zero. Again, the variation of the objective function, δJ should not depend on the variation of the unknown, δu. Hence the terms containing δu should be zero.

Vanishing the integrands containing δu we get the following equations for the adjoint function λ.

$$\nabla_u^+ L\lambda + \frac{\partial f}{\partial u} = 0 \qquad (2.394)$$

$$\lambda = 0 \quad when \quad t = t_f \qquad (2.395)$$

$$\nabla_u^+ L_{UB}\lambda + \frac{\partial f}{\partial u} = 0 \quad on \quad (\Gamma_{UB}) \qquad (2.396)$$

$$-\nabla_u^+ L_{LB}\lambda + \frac{\partial f}{\partial u} = 0 \quad on \quad (\Gamma_{LB}) \qquad (2.397)$$

Hence Equation (2.392) reduces to

$$\delta J = \left(\delta p, \nabla_p^+ L\lambda + \frac{\partial f}{\partial p}\right)_{\Omega,T} + (\delta p, \nabla_p^+ L_{UB}\lambda)_{\Gamma_{UB},T} - (\delta p, \nabla_p^+ L_{LB}\lambda)_{\Gamma_{LB},T} \qquad (2.398)$$

Therefore for any unknown parameter p we can obtain the following equation

$$\frac{\partial J}{\partial p} = \int_{t=t_0}^{t_f} \int_{\Omega} \left(\nabla_p^+ L\lambda + \frac{\partial f}{\partial p}\right) d\Omega \, dt \qquad (2.399)$$

From the definition of δJ

$$\frac{\partial J}{\partial p} = \int_{t=t_0}^{t_f} \int_{\Omega} J'_p \, d\Omega \, dt \qquad (2.400)$$

Comparing Equations (2.399) and (2.400) we have

$$J'_p = \nabla_p^+ L\lambda + \frac{\partial f}{\partial p} \qquad (2.401)$$

where the boundary integral terms in (2.393) are assumed to be zero. Equation (2.401) is called the gradient of the functional with respect to the parameter p. Equations (2.394-2.397) is the applicable system for determining the function λ.

2.7.6 Adjoint Operations

It is possible to find the transpose of the adjoint matrices $\nabla_u^+ L$,$\nabla_p^+ L$,$\nabla_u^+ L_B$ and $\nabla_p^+ L_B$ by following certain symbolic rules. For any matrix A we define $A^+ = (A^*)^T$, where asterisk denotes the adjoint operation and superscript T denotes transpose operator. Adjoint operation rules for differential operators can be derived from Green's formula. Some of these rules of operation are given in the table below.

Table 2.1: Adjoint Operation Rules for Differential Operators

Element of ∇L	Element of $\nabla^* L$
$F.$	$F.$
$F\frac{\partial}{\partial t}.$	$-\frac{\partial}{\partial t}(F.)$
$\frac{\partial}{\partial t}(F.)$	$F - \frac{\partial}{\partial t}.$
$\nabla(F\nabla.)$	$\nabla(F\nabla.)$
$\nabla(K\nabla.)$	$\nabla(K\nabla.)$
$V(\nabla.)$	$-\nabla(V.)$
$\nabla(V.)$	$-V(\nabla.)$
$\nabla(F\nabla G.)$	$-F\nabla G\nabla.$
$\nabla(K\nabla G.)$	$-K\nabla G\nabla.$
$\nabla[K\nabla(F.)]$	$F\nabla(K\nabla.)$

Some of the adjoint operator rules for elements of the boundary operator ∇L_B are given in Table 2.7.6.

The steps of deriving the adjoint equations can be summarized as follows:

1. Find gradient operator matrices $\nabla_u L, \nabla_p L, \nabla_u L_{LB}, \nabla_u L_{UB}, \nabla_p L_{LB}$ and $\nabla_p L_{UB}$ using (2.376) and (2.377).
2. From (2.378) and (2.379) calculate $\nabla_u^* L, \nabla_p^* L, \nabla_u^* L_B$ and $\nabla_{p^*} L_B$ using adjoint operation rules, and then obtain $\nabla_u^+ L, \nabla_p^+ L, \nabla_u^+ L_B, \nabla_{p^+} L_B$ by transposition.
3. Obtain the adjoint Equation (2.394)
4. Obtain the final and boundary conditions of the adjoint problem (2.395-2.397).

Table 2.2: Adjoint Operation Rules for Elements of the Boundary Operator

Element of ∇L_B	Element of $\nabla^* L_B$
$(V.)n$	0
$(F\nabla.)n$	$(F\nabla.)n$
$(K\nabla.)n$	$(K\nabla.)n$
$[K\nabla(F.)]n$	$(FK\nabla.)n$

5. Obtain all partial derivatives of the cost function J with respect to the parameters (2.401).

2.7.7 Stopping Criterion

If the problem involves no measurement errors, the traditional condition specified as

$$J^{n+1}(p_1, p_2 \cdots p_M) < \epsilon \tag{2.402}$$

where ϵ is a small specified number, can be used as the stopping criterion. However, the recorded data contains measurement error; as a result, the inverse solution will respond to the perturbed input data. The estimated parameters consequently will exhibit oscillatory behavior as the number of iterations is increased. The computational experience has shown that it is advisable to use the discrepancy principle for terminating the iteration process in the conjugate gradient method. It is assumed that the standard deviations of measurement errors for unknown variables $u_1, u_2 \cdots u_N$ are equal in magnitude and are given by σ. Then the discrepancy principle that establishes the stopping criterion ϵ can be obtained from Equation (2.367) as

$$\int_{t=0}^{t_f} \int_{\Gamma_{LB}}^{\Gamma_{UB}} \sigma^2 \, d\Omega \, dt \equiv \epsilon^2 \tag{2.403}$$

Then the stopping criterion is taken as

$$\left|J(p_1^{n+1}, p_2^{n+1} \cdots p_M^{n+1})\right| < \epsilon \tag{2.404}$$

where ϵ is determined from Equation (2.403).

2.7.8 Computational Procedure

The iterative computational procedure for the conjugate gradient method for the general problem can be summarized as follows (assume all the parameters p_1, $p_2 \cdots p_M$ are known at nth iteration).

Step 1: Solve the direct problem (2.358-2.364) and compute unknown variables u_1, $u_2, \cdots u_N$.

Step 2: Solve the adjoint problem (2.394-2.397) and obtain adjoint variables λ_1, $\lambda_2, \cdots \lambda_N$.

Step 3: Compute gradients J'^n_{p1}, J'^n_{p2} $\cdots$and J'^n_{pM} using equation (2.401).

Step 4: Compute ν^n_{p1},ν^n_{p2} $\cdots$ and ν^n_{pM} from Equation (2.371). Then estimate the directions of descent, P^n_{p1},P^n_{p2} $\cdots$ and P^n_{pM} using Equation (2.370).

Step 5: Solve the sensitivity problems (2.372-2.375) to obtain δu.

Step 6: Compute search step sizes β^n_{p1}, β^n_{p2} $\cdots$ and β^n_{pM}.

Step 7: Compute new set of parameters ${p_1}^{n+1}, {p_2}^{n+1}, \cdots$ and ${p_M}^{n+1}$ from Equation (2.369).

Step 8: Repeat the above calculational procedure until the discrepancy principle defined by Equation (2.404) is satisfied.

Chapter 3

SOLUTION OF HEAT CONDUCTION EQUATION

Numerical results obtained using the inverse technique of Chapter 2 are represented below for one dimensional heat conduction equations.

3.1 Opening Remarks

The accuracy of parameter estimation by the inverse technique depends on variety of factors in addition to the measured temperature itself, other quantities of importance are time and position measurement, specimen geometry and boundary conditions particularly of the heat flux and heat loss variety. In the present study, uncertainties in the measured temperature alone have been considered. Other factors that influence the prediction include temperature measurement at discrete and data lugging with the finite sampling scheme. The fact that the series of direct problems appearing in the inverse procedure are also to be numerically solved, contributes to the errors in parameter estimation.

It has now been established that inverse techniques are mathematically illposed in the sense that they amplify errors in the input data. This extreme sensitivity to errors manifest in the form of higher errors in predictions as well as possible delay in convergence when supplied with an inappropriate initial guess. An unexpected consequence is loss of size convergence, namely the absence of convergence in the limit of small space and time steps.

The results discussed in the present and later chapters have to be interpreted in the light of the comments made above.

3.2 Numerical Issues

Direct problems arising from the inverse calculation have been solved by a control volume finite difference method (Appendix A). The finite difference equations have been solved by the TDMA algorithm. When the equation is nonlinear, Picard iterations are required.

3.3 Estimation of 'K' from Steady State Heat Conduction Problem

The mathematical formulation for estimating thermal conductivity from steady state heat conduction equation has been in Section 2.2. In parameter estimation a detailed examination of the sensitivity coefficients can a provide considerable insight into the calculation. These coefficients can show possible areas of difficulty and also lead to an improved experimental design. The sensitivity coefficient is defined as the first derivative of the dependent variable with respect to the unknown parameter. If the sensitivity coefficients are either small or correlated with one another, the estimation problem becomes very sensitive to measurement errors. In Figure (3.1) the distribution of sensitivity of temperature to thermal conductivity as a function of distance x is shown. The magnitude of the sensitivity becomes zero at $x = 0$. The sensitivity increases with distance up to $x \approx 0.5$. It starts decreasing beyond $x = 0.5$. Finally it goes to zero at $x = 1$.

The foregoing results have an implication for the design of the experiment. Since the sensitivity is very small at the points close to the boundaries, measurements should be taken at the points which are close to the mid-point of the slab.

To illustrate the validity and accuracy of the conjugate gradient method in predicting thermal conductivity $K(T)$, we consider a specific example. Here the exact functional form of thermal conductivity is assumed to be second-order polynomial with temperature as

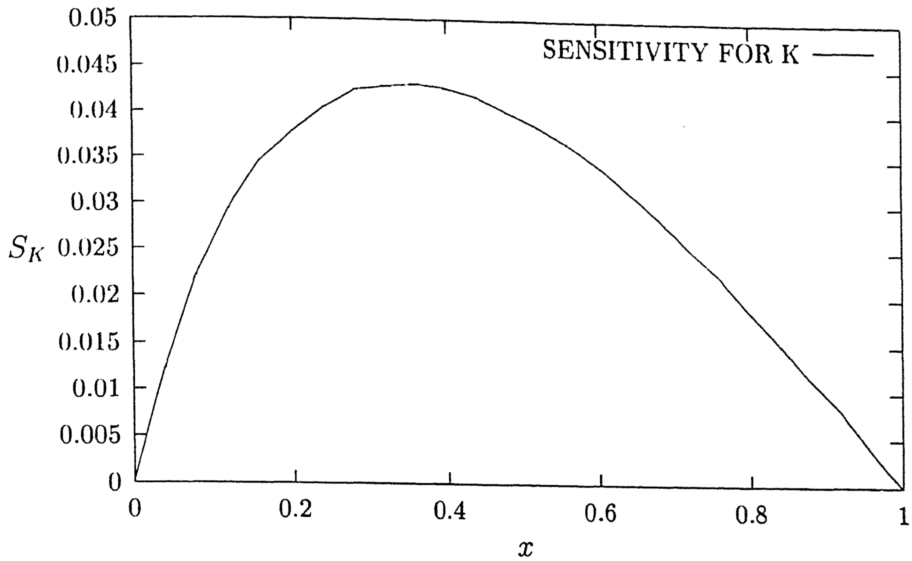

Figure 3.1: Distribution of sensitivity for K with space for steady state problem

the dependent variable, i.e.

$$K(T) = a_0 + a_1 \times T + a_2 \times T^2 \tag{3.1}$$

where the constants a_0, a_1 and a_2 are taken as 10.0, −0.5 and −0.1 respectively. The two boundaries are subjected to constant temperatures, $T_1 = 5.0$ and $T_2 = 1.0$ respectively. The grid size is taken as $\Delta x = 0.01$ in the finite difference calculations; thermocouple spacing Dx equals the finite-difference spacing Δx.

3.3.1 Inversion of Error-Free Data

Consider first the inversion of a hypothetical data set assumed to be entirely free of error in temperature measurements. The temperature distribution from the solution of the direct problem (2.12- 2.14). While simulating measurement temperatures, the form of exact $K(T)$ is used in the direct problem. Thus the problem is nonlinear and the iterative technique is needed for its solution. In the inverse calculation, the thermal conductivity takes the form of $K(x)$. The problem thus becomes linear and the estimated temperature can be calculated directly. The objective of this section is to show the applicability of the inverse procedure in finding $K(T)$ accurately with no prior information on the functional form of the unknown quantities, the so-called function estimation. One of

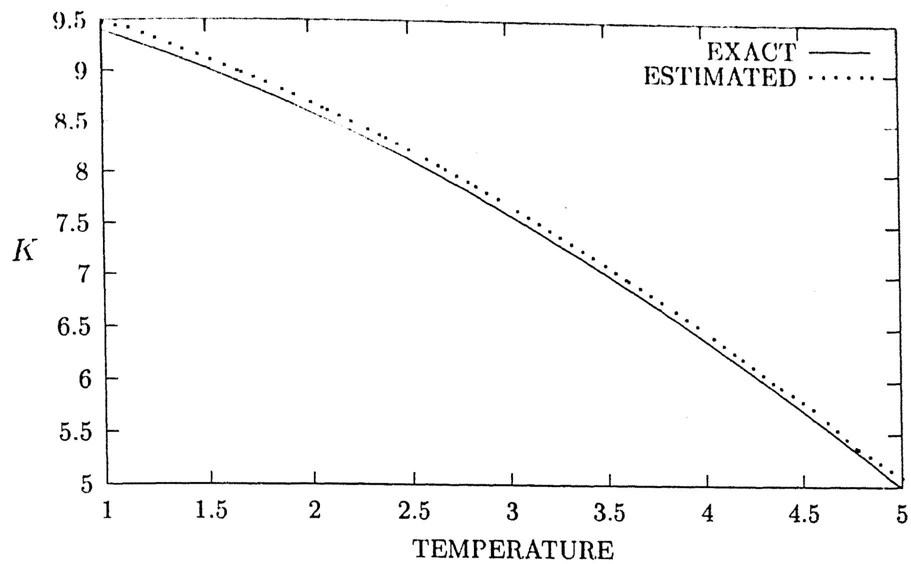

Figure 3.2: Exact and estimated values of $K(T)$ when $SD = 0$

the advantages of using the conjugate gradient method is that the initial guesses of the unknown quantities can be chosen arbitrarily. This advantage could not be exploited in the present study. This is due to the fact that if $K(T)$ satisfies Equation (2.12), $\alpha K(T)$ also satisfies Equation (2.12). Here α is a scalar quantity. If the initial guess of $\hat{K}(x)$ is very far from the actual conductivity, the estimated conductivity will differ from the actual conductivity. But the estimated and exact functions are parallel to each other. In the test case considered here, the initial guess of $\hat{K}(x)$ used to begin the iteration was taken as $\hat{K}^0(x) = 4$. The estimated function $K(x)$ obtained using exact input data is shown in Figure 3.2. The value of the functional J decreased to less than 10^{-8} after iterations. number of iterations is increased.

3.3.2 Effects of Data Errors

In order to compare the results for situations involving random measurement errors, we assume normally distributed uncorrelated errors with zero mean and a constant standard deviation superimposed on the input data. The simulated inexact measurement data Y can be expressed as

$$Y = Y_{exact} + \omega \times SD \tag{3.2}$$

where Y_{exact} is the solution of the direct problem with the exact form of $K(T)$, SD is the

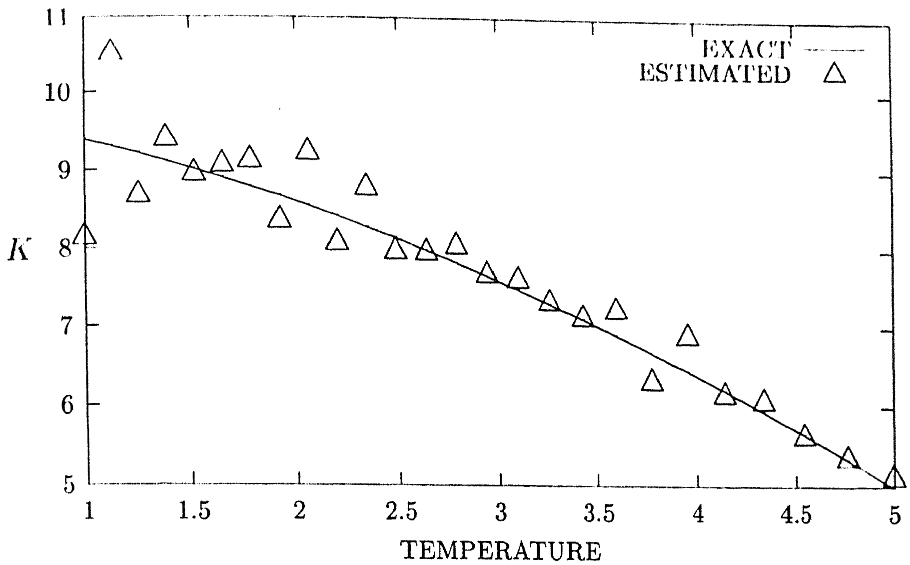

Figure 3.3: Exact and estimated values of $K(T)$ when $SD = 0.005$

standard deviation of the measurements, and ω is a random variable that is generated by subroutine RAND and will be within -2.576 t0 2.576 for a 99% confidence bounds. The dimensionless measured temperature with an error corresponding to $\sigma = 0.001$ was obtained according to Equation (3.2). This represents an error in temperature of about 0.02%. The inverse solution using these inexact measurements are shown in Figure 3.3.

Table 3.1: The convergence parameters for steady state heat conduction

Measurement error, σ	Stop Criterion $\lvert J^{n+1} - J^n \rvert$	Number of iterations	CPU time (s)	K_{rms}
0.000	10^{-5}	10	0.23	0.085
0.005		76	0.52	0.262

3.4 Determination of K and C from a Transient Experiment

In the previous section we only the thermal conductivity has been estimated from the steady state data. In this section the simultaneous estimation of temperature-dependent thermal conductivity and heat capacity has been discussed. No prior information is used for the functional forms of the unknown thermal conductivity and heat capacity in the present study. Two different boundary conditions have been considered for comparison.

3.4.1 Non-zero Fluxes at the Boundaries

The mathematical formulation for simultaneously measuring temperature-dependent thermal conductivity and heat capacity from a transient heat conduction experiment with nonzero fluxes at the boundaries has been presented in Section 2.3. To illustrate the validity and accuracy of the conjugate gradient method in simultaneously predicting $K(T)$ and $C(T)$ with inverse analysis from the knowledge of transient temperature records, a specific example is considered. Here the exact functional form of thermal conductivity and heat capacity are taken as second order polynomials with temperature as the dependent variable, i.e.

$$K(T) = a_0 + a_1 \times T + a_2 \times T^2 \tag{3.3}$$

$$C(T) = b_0 + b_1 \times T + b_2 \times T^2 \tag{3.4}$$

where the constants a_0, a_1 and a_2 are taken as 6.0, -0.15 and -0.015 respectively, and the constants b_0, b_1 and b_2 are 1.2, 0.1 and 0.01 respectively. The medium has initial temperature $T_0 = 1.0$, when $t > 0$. The two boundaries at $x = 0$ and $x = 1$ are subjected to constant heat fluxes, $q_1 = 17.0$ and $q_2 = 6.0$ respectively. To compare the results for situations involving random errors, we assume normally distributed uncorrelated errors with zero mean and constant standard deviation. The simulated inexact measurement data $Y(x, t)$ can be expressed by

$$Y(x,t) = Y_{exact}(x,t) + \omega\sigma \tag{3.5}$$

While generating simulated measurement temperature Y, exact $K(T)$ and $C(T)$ are used in the direct problem and thus the problem is nonlinear and the iterative technique in

needed for its solution. However, in the inverse calculation, the thermal conductivity and heat capacity exist in the form of $K(x,t)$ and $C(x,t)$, so the problem becomes linear and the estimated temperature can be calculated directly.

The space and time increments are taken as $\Delta x = 0.05$ and $\Delta t = 0.02$ respectively, in the finite difference calculations; the total measurement time is chosen as $t_f = 1.2$. We assume that the thermocouples are placed at a regular interval Dx and temperatures are measured at these thermocouple points at a regular interval of time Dt. In the entire calculations we assume that the thermocouple spacing Dx equals the finite-difference spacing Δx. The measurement time step Dt is taken the same as Δt.

One of the advantages of using the conjugate gradient method is that the initial guesses of the unknown quantities can be chosen arbitrarily. However, this is not valid in this problem. The reason is because two unknown functions, $K(x,t)$ and $C(x,t)$, are to be estimated simultaneously by using only the measurement temperature $Y(x,t)$, which implies that the estimated temperature $T(x,t)$ obtained by utilizing any combination of $K(x,t)$ and $C(x,t)$ could possibly equal $Y(x,t)$, but the estimated thermal properties are not correct ones.

In order to restrict the region of search directions to obtain the correct inverse solutions, a good initial guess of either thermal conductivity, $K(x,t)$, or heat capacity, $C(x,t)$, should be given prior to the inverse calculations. Good initial guesses for heat capacity can be obtained from from the following energy balance equation

$$[q(t_{j+1}) - q(t_j)]\Delta t = \int_{x=0}^{x=1} \bar{C}(t_j)[T(x,t_{j+1}) - T(x,t_j)]dx \tag{3.6}$$

where $q = q_1 - q_2$; j represents the time index; Δt denotes the time increment for use in the finite-difference calculation and $\bar{C}(t_j)$ is an averaged value for heat capacity at $t = t_j$.

The variation of the sensitivity coefficient of thermal conductivity to temperature as a function of time is shown in Figure 3.4 . The sensitivity coefficient is zero at $t = 0$. The sensitivity increases with time, but the sensitivity at $x = 1$ is smaller compared to that at $x = 0$ for time t ¿0. Since the sensitivity of K is small for small time, the estimated thermal conductivity is inexact. Therefore it is recommended that the few initial time steps be ignored in the inverse calculations.

The variation of the sensitivity coefficient of heat capacity to temperature as a

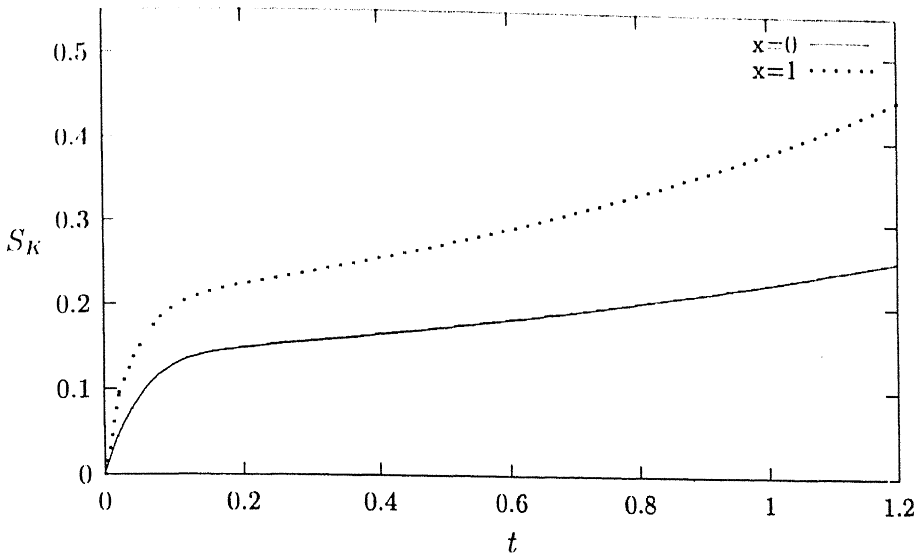

Figure 3.4: Variation of sensitivity coefficient for K to temperature as a function of time

function of time is shown in Figure 3.4.1. The sensitivity is initially zero and its magnitude increases with time. Figure 3.4.1 also shows that the sensitivity coefficient does not vary with x. It is also observed that the magnitude of the sensitivity coefficient of C is greater than that of K. One can then expect reconstruction errors in C to be smaller than in K.

The foregoing results have several implications for the design of experiments. The pattern of sensitivity coefficients indicates that the information obtained from the inverse calculations are less reliable for the initial time steps. It also indicates the results for K are less critical at the points near $x = 0$.

In all the test cases considered here, the initial guesses of $K(x,t)$ used to begin the iteration are taken as 4.5. The estimated functions $K(x,t)$ and $C(x,t)$ with $\sigma = 0.0$, $\sigma = 0.005$ and $\sigma = 0.01$, are shown in Figures (3.6-3.13) The value of the functional J obtained with $\sigma = 0$ can be reduced to a very small number as the number of iterations is increased. The dimensionless measured temperature with $\sigma = 0.005$ and $\sigma = 0.01$ are obtained according to Equation (3.5). In order to show $K(T)$ and $C(T)$ explicitly as functions of temperature, T, the thermal conductivity and heat capacity at $x = 0.2, 0.4, 0.6$ and 0.8 with $\sigma = 0, 0.005$ and 0.01 are shown in Figures (3.6-3.13). An increase in the measurement errors causes a drop in the accuracy of the inverse solution. For $\sigma = 0.01$, the noise level in the reconstructed thermal conductivity function is seen to

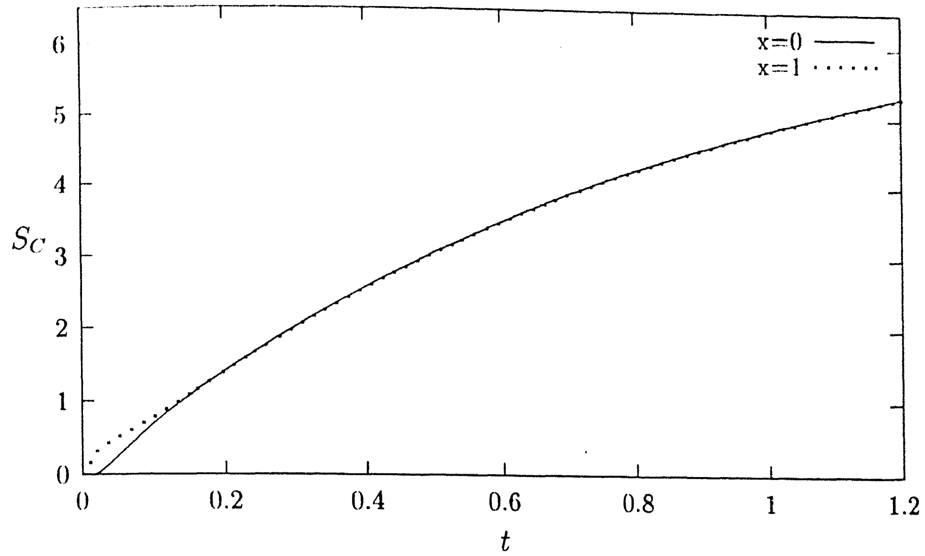

Figure 3.5: Variation of sensitivity coefficient for C to temperature as a function of time

be quite high. [Remark: The thermal conductivity reconstruction at $\sigma = 0.01$ was seen to be meaningful after filtering.]

Figures (3.6-3.13) show that the estimated values of conductivity and heat capacity deviate from the actual values for the few initial time steps. The reason is that at interior points temperature gradients are initially small. From Equations (2.94-2.95) it is clear that if the temperature gradient is small, the gradient of the functional, $J'(x,t)$ becomes small. That implies that the estimated values of the parameters are close to the guess values at the points of very low temperature gradients.

It is to be noted that $J'(x,t_f)$ always equals zero since $\lambda(x,t_f) = 0.0$. Therefore the estimated values of the unknown functions, $K(x,t)$ and $C(x,t)$ for final time are the same as the initial guess values $K^0(x,t_f)$ and $C^0(x,t_f)$ respectively. There are two methods to avoid such a singularity. One is to use modified conjugate gradient method and the second is to record data for a little longer time compared to the actual period of interest. In the present study we applied the second method for solving the gradient equations.

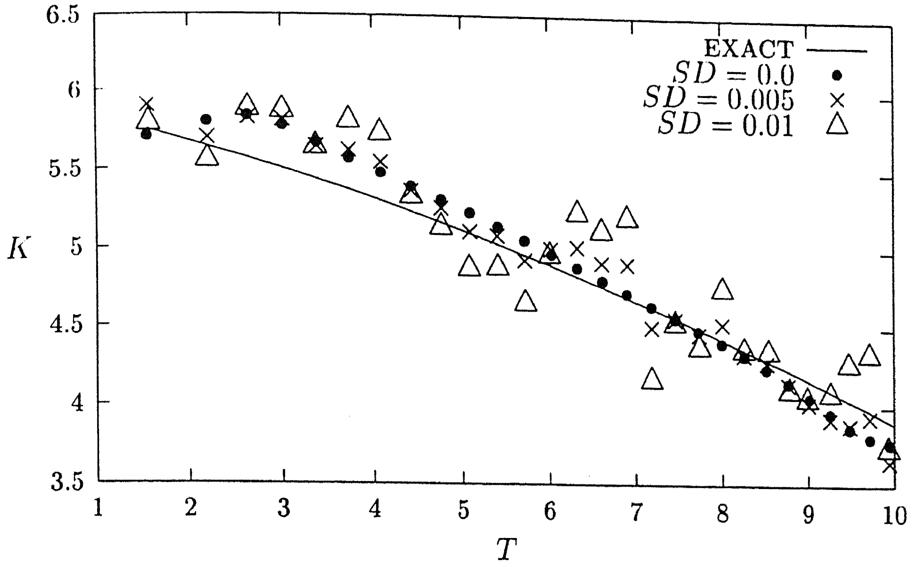

Figure 3.6: Exact and estimated values of $K(T)$ at $x = 0.2$

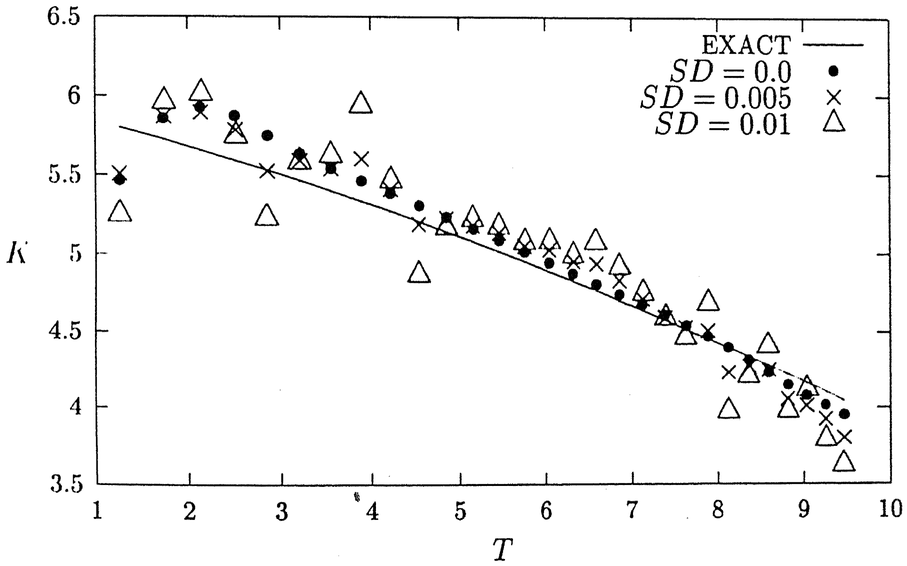

Figure 3.7: Exact and estimated values of $K(T)$ at $x = 0.4$

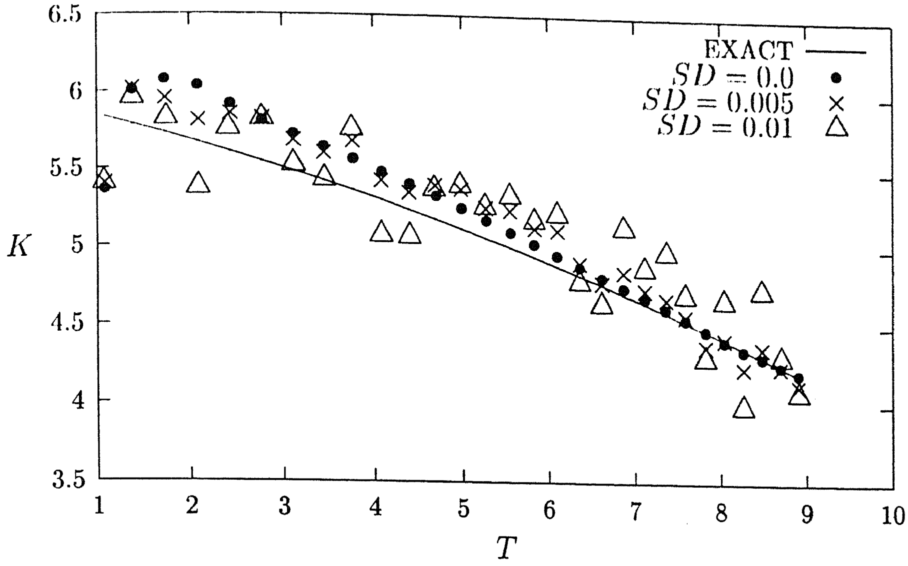

Figure 3.8: Exact and estimated values of $K(T)$ at $x = 0.6$

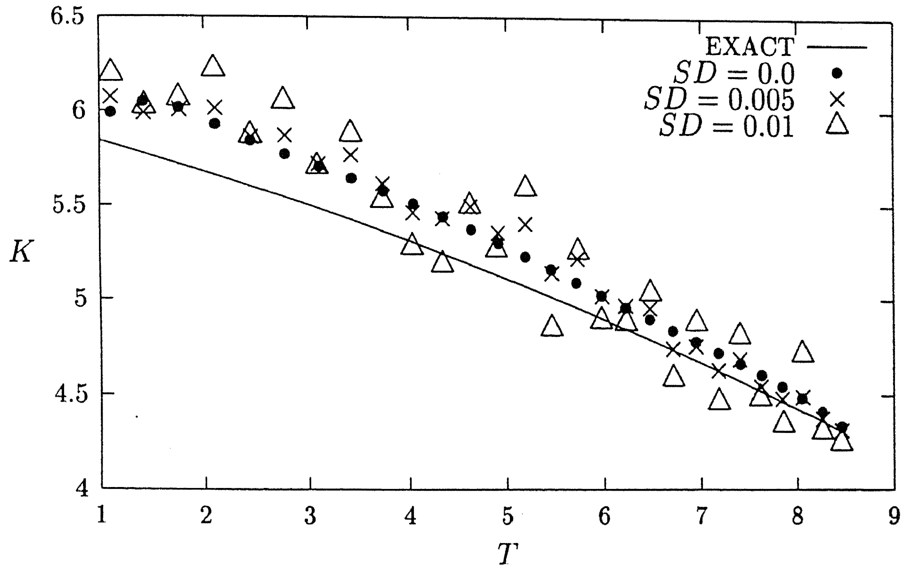

Figure 3.9: Exact and estimated values of $K(T)$ at $x = 0.8$

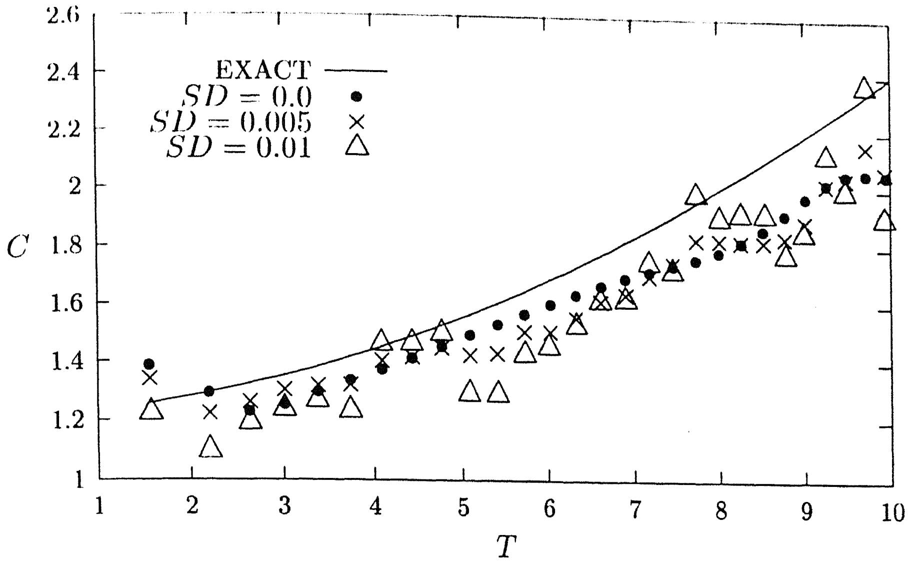

Figure 3.10: Exact and estimated values of $C(T)$ at $x = 0.2$

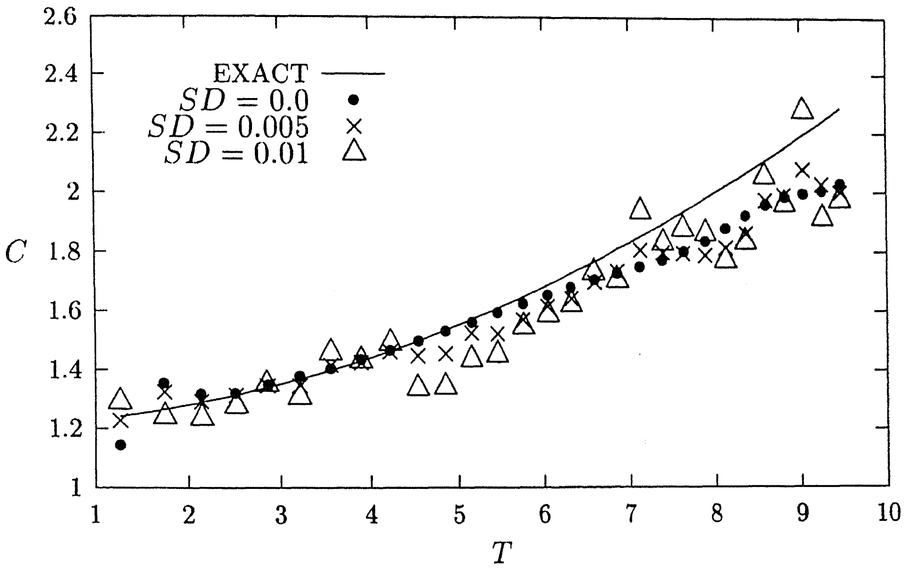

Figure 3.11: Exact and estimated values of $C(T)$ at $x = 0.4$

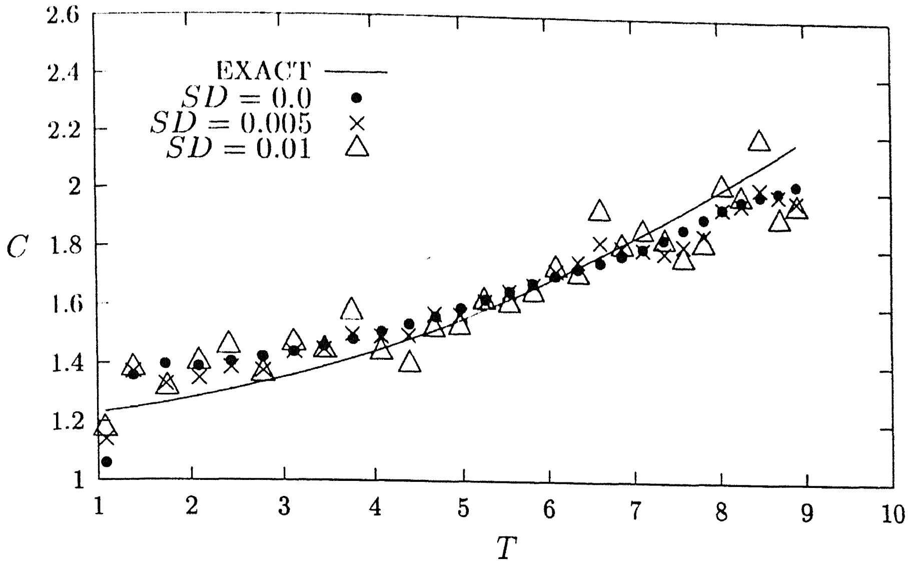

Figure 3.12: Exact and estimated values of $C(T)$ at $x = 0.6$

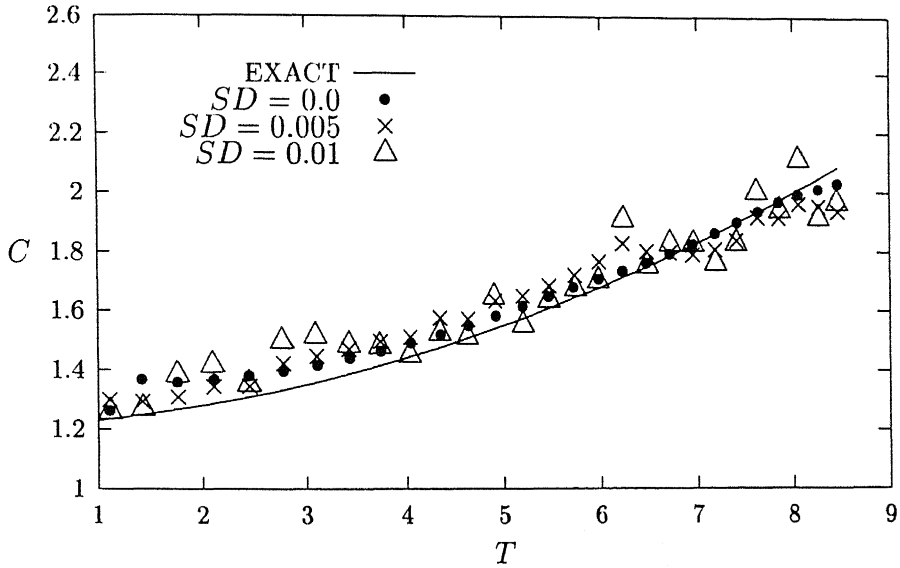

Figure 3.13: Exact and estimated values of $C(T)$ at $x = 0.8$

3.4.2 Non-zero Flux at One Boundary and Zero Flux at Oth

A special case of the flux-flux boundary conditions arises when one of the fluxes is ze This configuration is indeed encpountered in practice and hence has been seperat treated. 2.3.1.

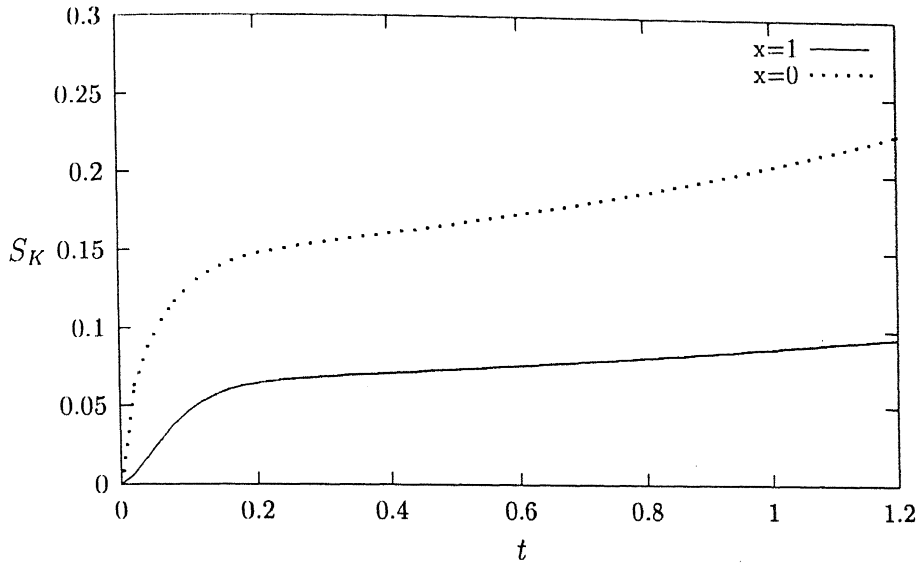

Figure 3.14: Variation of the sensitiviy coefficient for K with to temperature as a functior of time

The sensitivity coefficient of the parameters K and C have been shown in the Figures (3.14 - 3.15). These figures show low sensitivity coefficients in the region of $t = 0$. The sensitivity become zero at $t = 0$. Therefore, the information given by inverse solution about the parameters will be different from the actual values for the few initial time steps. To obtain the actual information we need to ignore a few initial time steps. Figure (3.14) also shows that the sensitivity of K decreases with increasing x. Hence the information obtained from the points close to the insulated end is less reliable. The comparison between Figures (3.14) and (3.15) shows that the sensitivity to K remains quite low compared to C. Hence the estimated values of C are expected to be more accurate as compared to K.

To illustrate the validity of the obove statements, we consider a specific example where the exact functional form of thermal conductivity and heat capacity are assumed

values K equal to 4.0 and measured temperature with $\sigma = 0$, $\sigma = 0.005$ and $\sigma = 0.01$ are shown in Figures (3.16 -3.23). As before the functional J obtained for $\sigma = 0$ can be decreased to a small number with increasing number of iterations. Figures (3.16-3.23) show that the estimated values of $\hat{K}(T)$ and $\hat{C}(T)$ deviate from actual values at the region of $T = 1.0$, i.e. for the few initial time steps. This is again due to the fact that temperature gradient becomes small at some interior points for few initial time steps. In Equation 2.82 we see that the adjoint function λ is zero at $t = t_f$. This indicates that the solution does not improve at the final time, t_f.

Table 3.2: The convergence parameter for the inverse heat conduction with non-zero fluxes

Measurement error, σ	Stop Criterion $\lvert J^{n+1} - J^n \rvert$	Number of iterations	CPU time (s)	K_{rms}	C_{rms}
0.000		97	12.18	0.2037	0.1308
0.005	10^{-6}	168	17.37	0.2687	0.1463
0.010		105	12.77	0.4170	0.2047

Table 3.3: The convergence parameter for the inverse heat conduction with non-zero flux at one boundary and zero flux at other

Measurement error, σ	Stop Criterion $\lvert J^{n+1} - J^n \rvert$	Number of iterations	CPU time (s)	K_{rms}	C_{rms}
0.000		82	9.62	0.4567	0.1178
0.005	10^{-6}	70	8.66	0.5045	0.1900
0.010		133	13.23	0.5744	0.3630

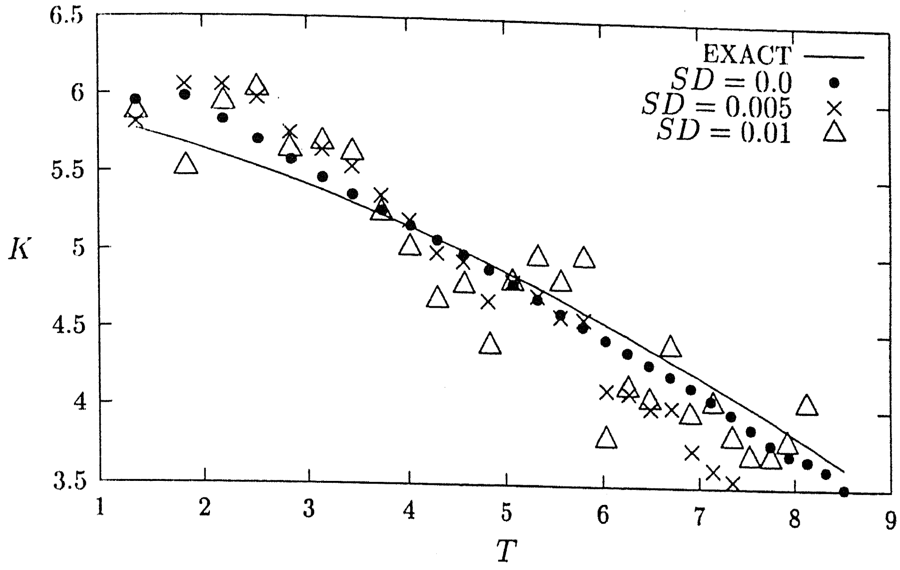

Figure 3.16: Exact and estimated values of $K(T)$ at $x = 0.2$

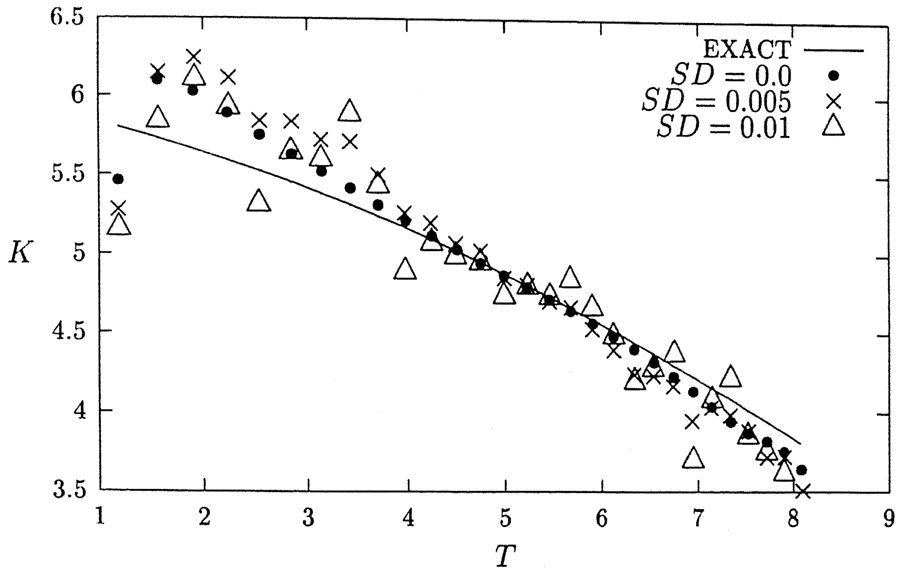

Figure 3.17: Exact and estimated values of $K(T)$ at $x = 0.4$

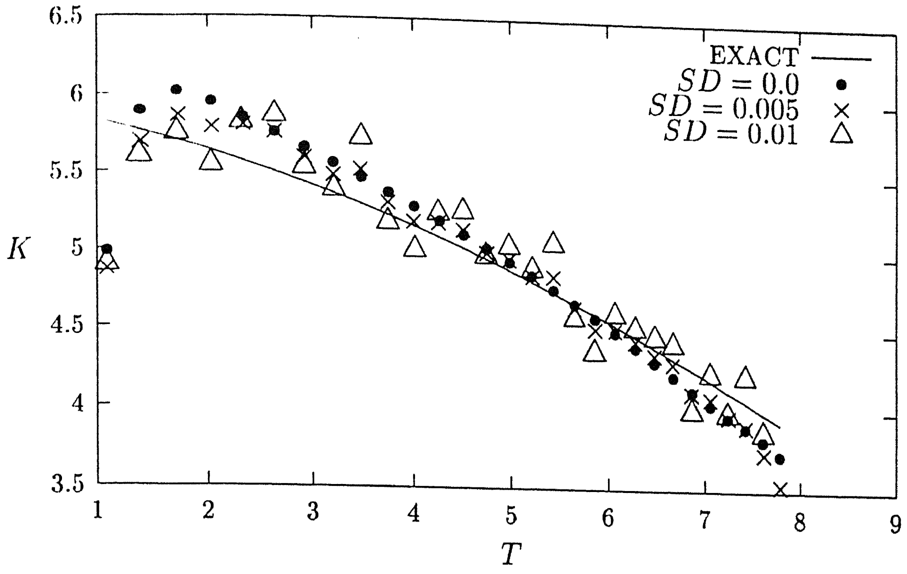

Figure 3.18: Exact and estimated values of $K(T)$ at $x = 0.6$

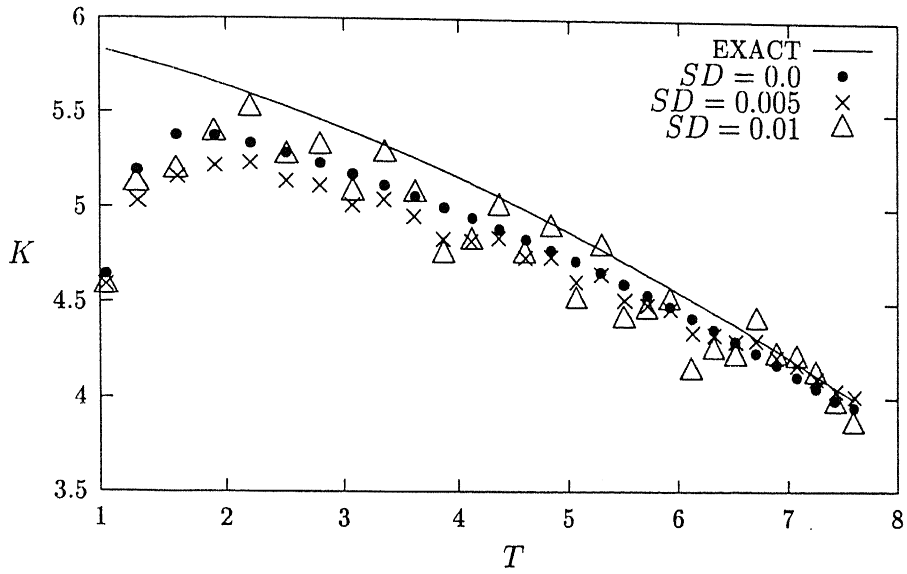

Figure 3.19: Exact and estimated values of $K(T)$ at $x = 0.8$

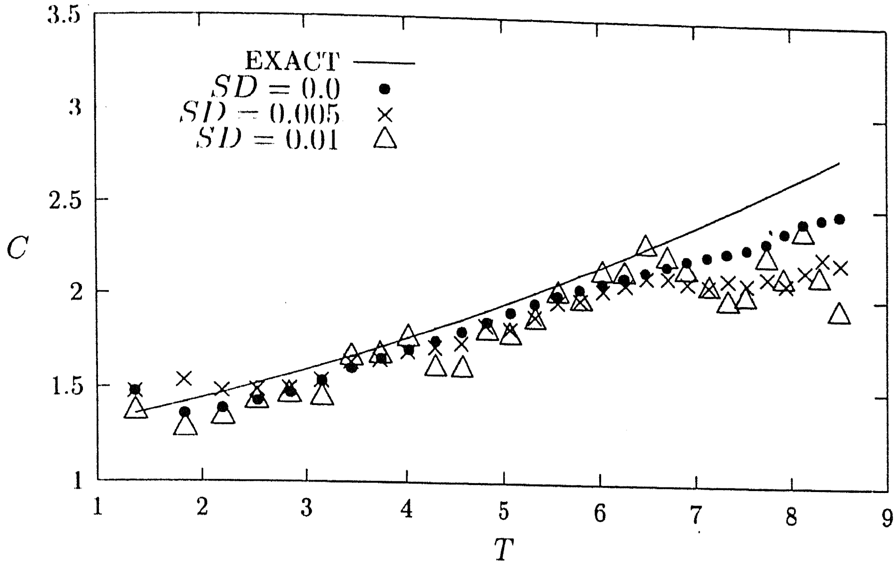

Figure 3.20: Exact and estimated values of $C(T)$ at $x = 0.2$

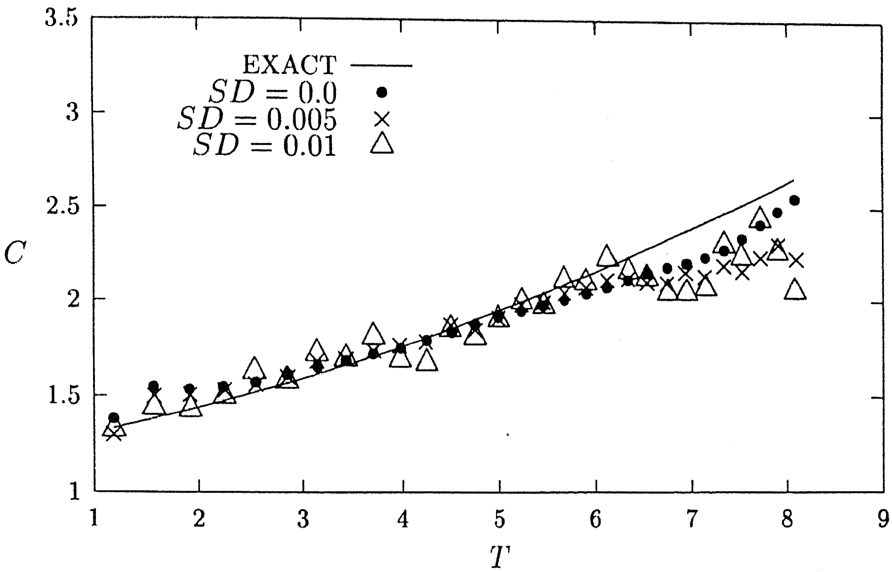

Figure 3.21: Exact and estimated values of $C(T)$ at $x = 0.4$

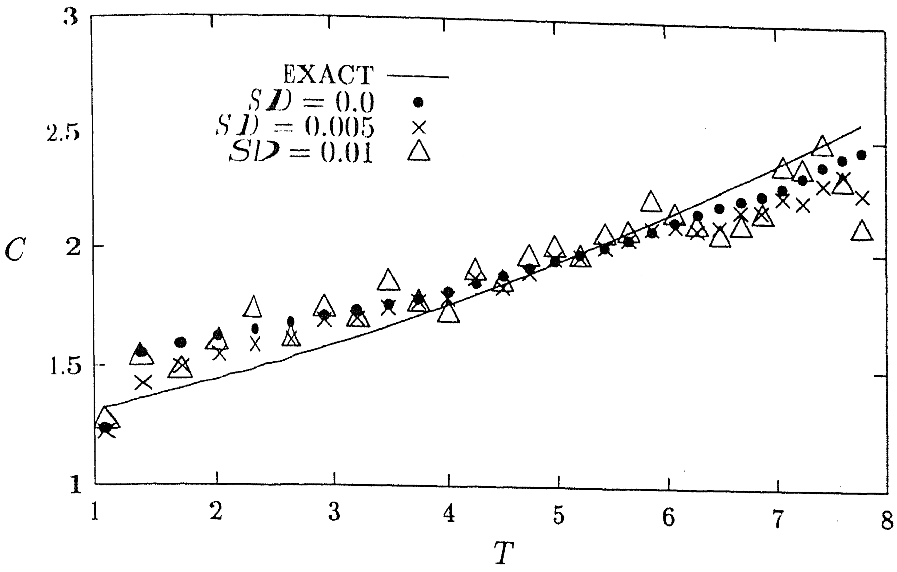

Figure 3.22: Exact and estimated values of $C(T)$ at $x = 0.6$

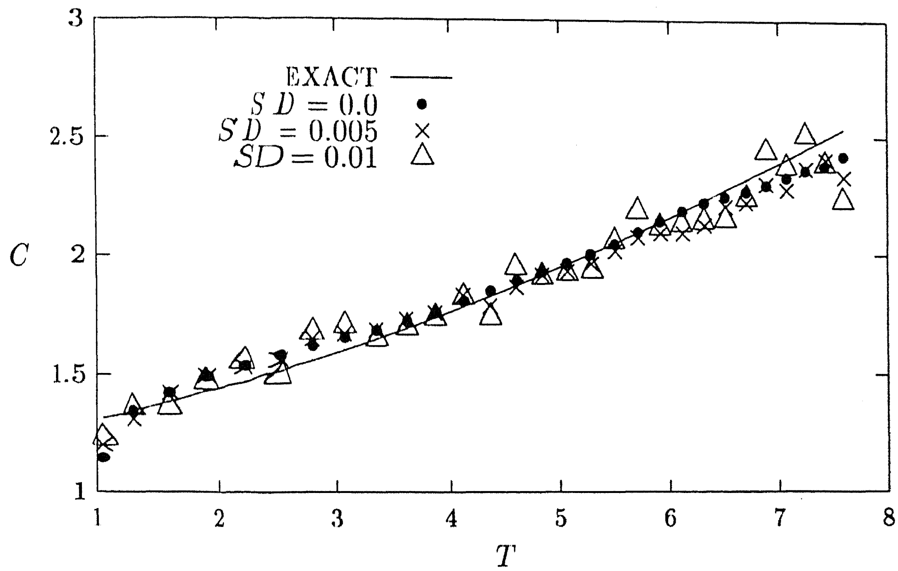

Figure 3.23: Exact and estimated values of $C(T)$ at $x = 0.8$

3.4.3 Flux-Temperature Boundary Conditions

There are a few essential differences between the flux-flux boundary conditions and flux-temperature boundary conditions, mainly arising from the possibility of a steady state in the latter. Inverse calculations with flux-temperature are discussed in the present section.

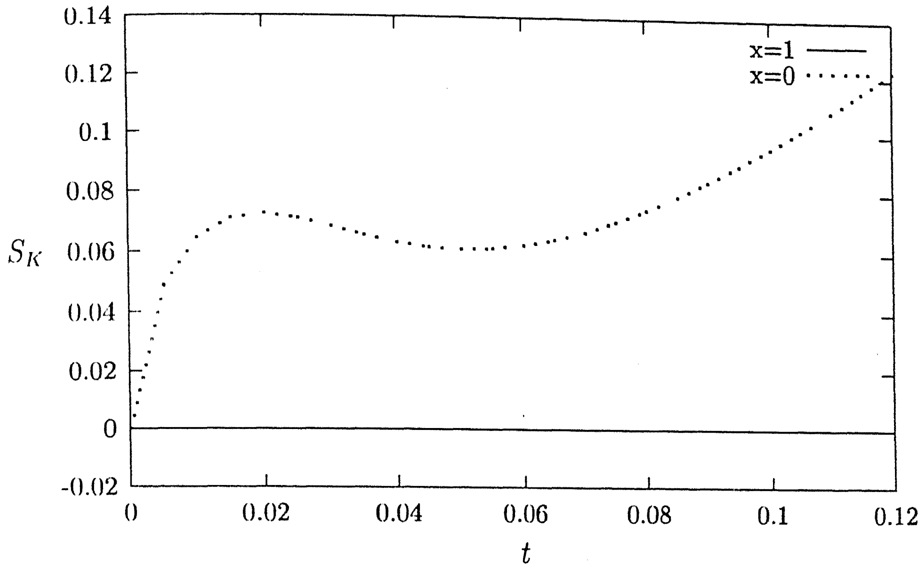

Figure 3.24: Variation of the sensitivity coefficient for K with to temperature as a function of time

The variation of sensitivities of K and C are shown in Figures (3.24 -3.25). The sensitivities of both K and C are identically zero at $x = 1$ (where temperature is prescribed). This implies that the solutions obtained from the inverse solution will deviate from the actual values at the points close to $x = 1$. The magnitudes of the sensitivities will also be in error for a few initial time steps. Therefore, the information given by the inverse problem is less reliable for the few initial time steps. The comparison between figures (3.24-3.25) shows that the sensitivity of parameter C is about one order of magnitude higher than that of K, except near $t = 0$. This indicates that the solution obtained for C is more accurate as compared to K.

To illustrate the validity of the above statements, we consider a specific example where the exact functional form of thermal conductivity and heat capacity are assumed to be second-order polynomials with temperature as the dependent variable, i.e.

$$K(T) = a_0 + a_1 \times T + a_2 \times T^2 \tag{3.9}$$

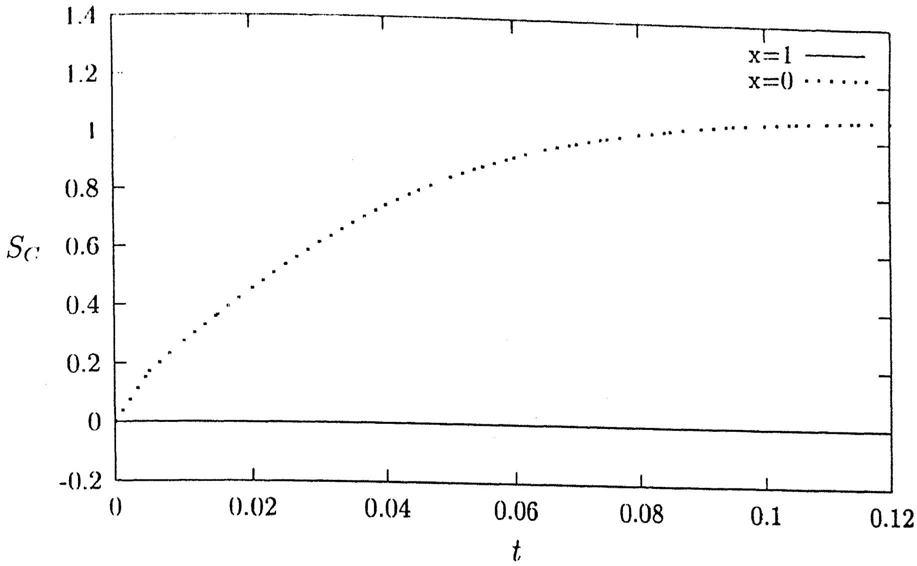

Figure 3.25: Variation of the sensitivity coefficient for C with to temperature as a function of time

$$C(T) = b_0 + b_1 \times T + b_2 \times T^2 \tag{3.10}$$

where the constants a_0, a_1 and a_2 for $K(T)$ are taken as 6.0, -0.15 and -0.05 respectively, and the constants c_0, c_1 and c_2 for C are chosen as 1.2, 0.15 and 0.05 respectively. The initial temperature is assumed to be 1.0. When $t > 0$, one boundary is subjected to a constant flux, $q_1 = 20.0$ and the other one is maintained at a constant temperature of $T_l = 3.0$.

The space and time increments are taken as $\Delta x = 0.025$ and $\Delta t = 0.001$ respectively, in the finite difference calculations. The total measurement time is chosen as $t_f = 0.12$. The thermocouple spacing Dx is assumed to be same as the finite difference spacing Δx. The measurement time step Dt is taken as Δt. The present problem is different from the previous two in the sense that the present problem reaches a steady state after some time. Using steady state data, C can not be determined from inverse calculation. For the flux-flux boundary conditions there is no steady state. In the present calculation, the fluxes are not known at the two boundaries, we cannot apply the equation (3.6) to estimate the initial guess of C. Therefore, we need to guess both the parameters, K and C arbitrarily. However, arbitrary guesses cannot be valid in the present case. The reason is because two unknown functions $K(x,t)$ and $C(x,t)$, are to be estimated simultaneously by using only the measurement temperature $Y(x,t)$. This implies that the estimated temperature

$T(x,t)$ obtained by utilizing any combination of $K(x,t)$ and $C(x,t)$ could possibly equal $Y(x,t)$, but the estimated thermal properties may not the correct ones. It is observed from the numerical experiments that the initial guesses of both thermal conductivity and heat capacity should be reasonably close to their average values. close to the range. In all the test cases considered here, the initial guesses of $\hat{K}(x,t)$ and $\hat{C}(x,t)$ used to begin the iteration are taken as $\hat{K}^0(x,t) = 5.5$ and $\hat{C}^0(x,t) = 2.0$ respectively.

The thermal conductivity and heat capacity at $x = 0.25$ and 0.5 with measurement errors $\sigma = 0$, 0.001 and 0.005 are presented in Figures (3.26-3.29). The comparison between the figures for estimated $\hat{K}(T)$ and $\hat{C}(T)$ shows that the estimated values of heat capacity are more accurate as compared to conductivity. Thus the results agree with predictions of the sensitivity analysis.

Table 3.4: The convergence parameters for flux-temperature boundary conditions

Measurement error, σ	Stop Criterion $\|J^{n+1} - J^n\|$	Number of iterations	CPU time (s)	K_{rms}	C_{rms}
0.000		24	2.73	0.3524	0.5517
0.005	10^{-6}	21	2.53	0.3549	0.5518
0.010		22	2.60	0.3970	0.5547

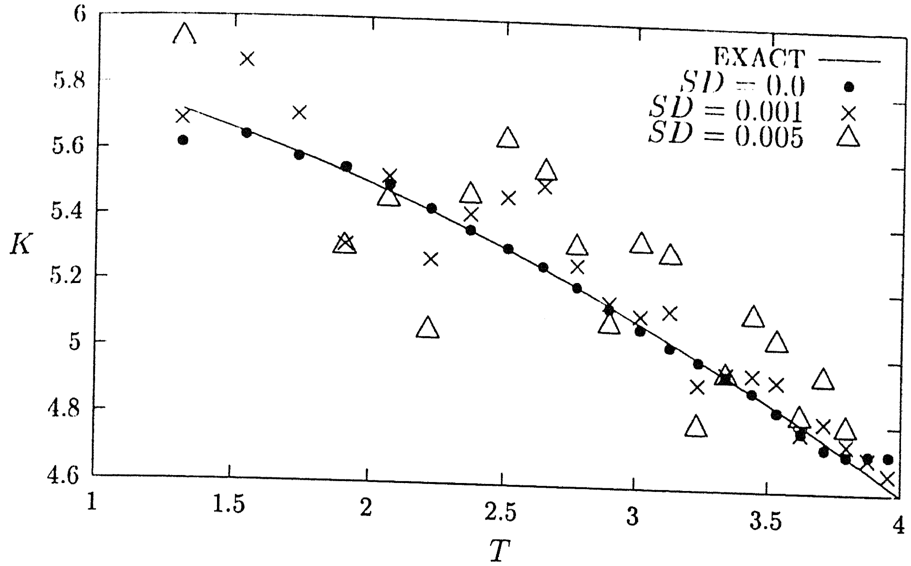

Figure 3.26: Exact and estimated values of $K(T)$ at $x = 0.25$

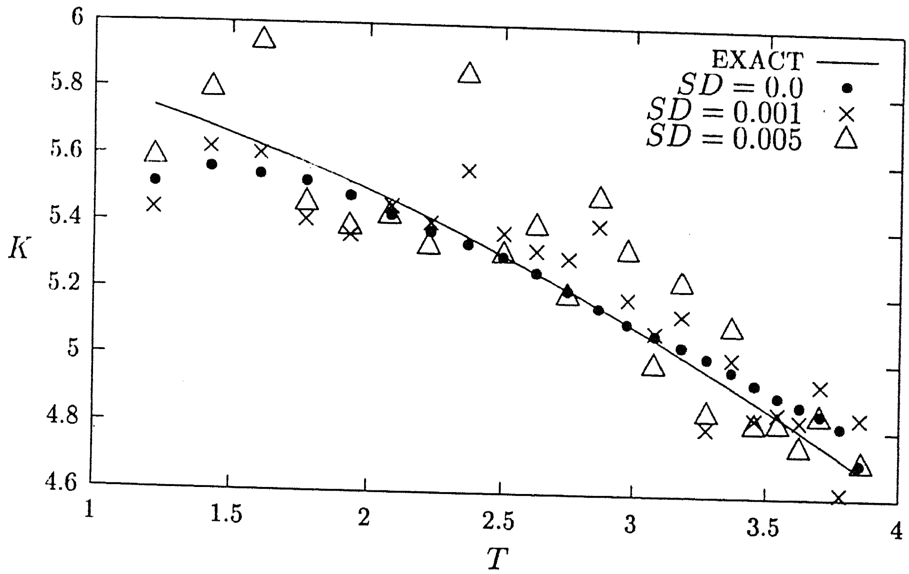

Figure 3.27: Exact and estimated values of $K(T)$ at $x = 0.5$

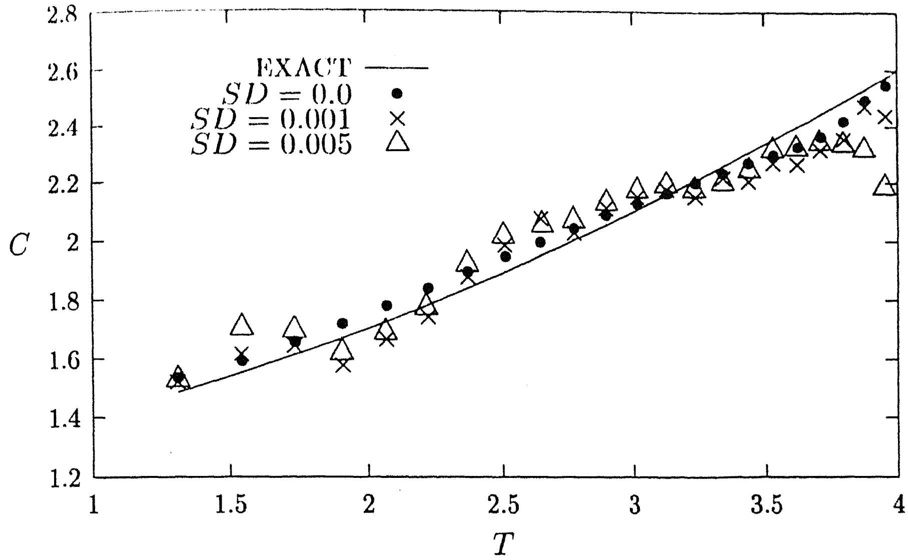

Figure 3.28: Exact and estimated values of $C(T)$ at $x = 0.25$

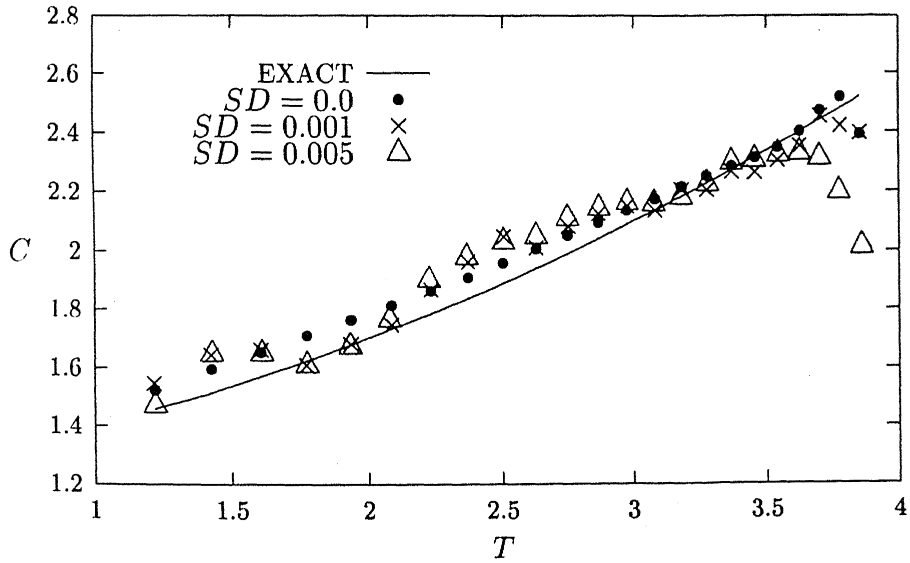

Figure 3.29: Exact and estimated values of $C(T)$ at $x = 0.5$

Chapter 4

COUPLED INVERSE PROBLEM

4.1 Introduction

In recent years, researchers and engineers working in the area of ground-water modeling are paying more attention to coupled problem. Examples are flow in saturated and unsaturated zones, heat and mass transport in aquifers with and without matrix deformation and geothermal reservoir evaluation. Coupled problems are also encountered in oil reservoirs and nuclear waste repositories.

The basic concepts and methods of solution for the coupled inverse problem are similar to the single variable inverse problem. However, there are several differences between them that make the coupled inverse problem more complex and challenging. First, the state variables of a coupled inverse problem often have different dimensions and uncertainties because they are measured by different instruments. Second, there are crossover effects between state variables and parameters. For example, relative permeability of oil and water depend upon water saturation, and water saturation depends on capillary pressure which is a function of oil and water pressures. Finally, there are many options in designing an experiment for the identification of unknown parameters.

The basic concepts and methods of solution for the coupled inverse problem have been discussed systematically in Chapter 2. Numerical results obtained with these techniques is presented below.

4.2 Estimation of Parameters for Coupled Equations without a Source Term

4.2.1 Steady State Problem

Sensitivity to Parameters

The methodology for developing expressions for use in simultaneously determining unknown parameters $K_1(T_1, T_2)$ and $K_2(T_1, T_2)$ has been described in Section 2.4.1. The boundary conditions used in this application are of flux-temperature type. The distributions of sensitivity coefficients of K_1 and K_2 over the domain are shown in Figures (4.1-4.2). The magnitude of the sensitivities are seen to decrease with x. Both the sensitivities become zero at $x = 1$. Therefore, the inverse solutions deviate from actual values at the points those are close to $x = 1$.

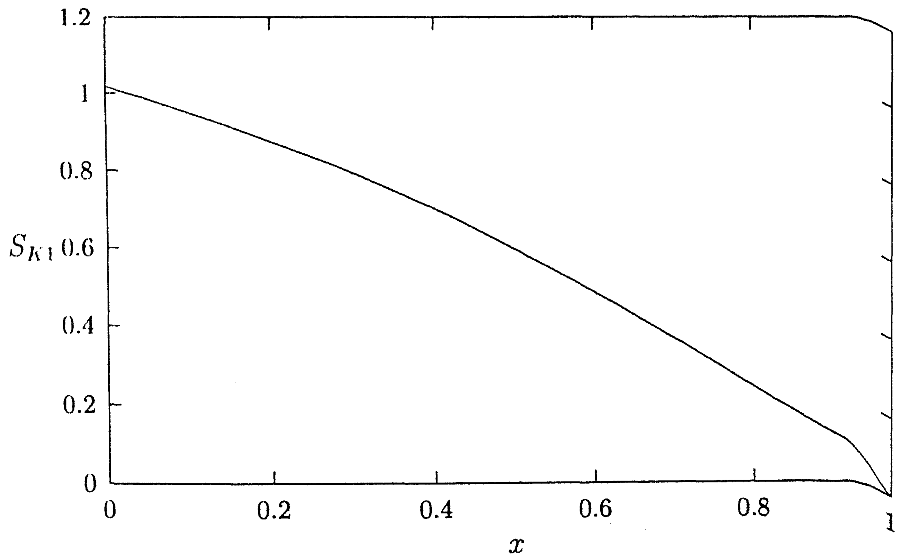

Figure 4.1: Variation of sensitivity coefficient of K_1 with distance

Solution of the Inverse Problem

To illustrate the validity and establish the accuracy of the conjugate gradient method in simultaneously predicting $K_1(T_1, T_2)$ and $K_2(T_1, T_2)$ by the coupled inverse analysis, we

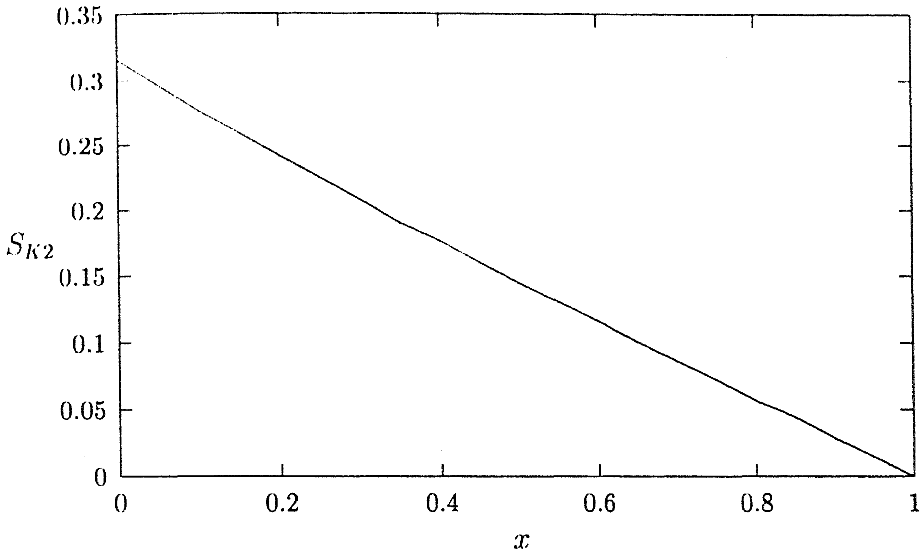

Figure 4.2: Variation of sensitivity coefficient of K_2 with distance

consider a specific example. Here the exact functional form of thermal conductivity and heat capacity are assumed to be second-order polynomials with $(T_1 - T_2)$ as the dependent variable, i.e.

$$K_1(T_1, T_2) = a_0 + a_1 \times (T_1 - T_2) + a_2 \times (T_1 - T_2)^2 \tag{4.1}$$

$$K_2(T_1, T_2) = b_0 + b_1 \times (T_1 - T_2) + b_2 \times (T_1 - T_2)^2 \tag{4.2}$$

where the constants a_0, a_1, a_2 and a_3 for K_1 are taken as 2.0, -0.15 and 0.15 respectively, and the constants b_0, b_1 and b_2 for K_2 are chosen as 3.5, 0.15 and -0.1 respectively. One boundary is subjected to constant fluxes q_1 and q_2, while T_1 and T_2 are kept constant at the other boundary. Here q_1 and q_2 are specified to be 5.0 and 2.0 respectively. The boundary values of both T_1 and T_2 are taken as 1.0.

The space increment is taken as $\Delta x = 0.05$ in the finite-difference calculations. The spacing Dx used for experiments is assumed to same as the finite difference spacing Δx.

The estimated functions $K_1(T_1 - T_2)$ and $K_2(T_1 - T_2)$, obtained when by exact measurement data, $\sigma = 0.0$, are shown in Figures (4.3) and (4.4) respectively. The value of the functional J obtained in such a case could be decreased to a very small number for increasing number of iterations.

In order to compare the results in the presence of random measurement errors, nor-

mally distributed uncorrelated errors with zero mean and a constant standard deviation have been assumed. The measurement errors for both K_1 and K_2 are assumed to have the same standard deviation, σ. The simulated inexact measurement data, Y_1 and Y_2, can be expressed as

$$Y_1 = Y_{1exact} + \omega_1 \sigma \tag{4.3}$$

$$Y_2 = Y_{2exact} + \omega_2 \sigma \tag{4.4}$$

where Y_{1exact} and Y_{2exact} are the solutions of the direct problem with the exact values of $K_1(T_1 - T_2)$ and $K_2(T_1 - T_2)$; ω_1 and ω_2 are random variables. The values of these random variables are -2.576 to 2.576 with 99% confidence interval. The dimensionless measured values Y_1 and Y_2 with error $\sigma = 0.001$ are obtained according to Equations (4.3) and (4.4).

From the numerical experiments it has been observed that the initial guesses of the parameters, K_1 and K_2 should be close to their average values. There are two possible reasons for the dependence of the inverse solutions with the initial guesses. First, two unknown functions K_1 and K_2, are to be estimated simultaneously by using Y_1 and Y_2. This requires that the estimated values T_1 and T_2 obtained by utilizing any combination of K_1 and K_2 could be equal to Y_1 and Y_2, but the estimated properties may not be correct. Second, Equations (2.131) and (2.132) show that if K_1 and K_2 satisfy the direct problem (2.131- 2.132), αK_1 and βK_2 also satisfy the equations for any scalars α and β. To circumvent these difficulties, the initial guesses of both $K_1(x)$ and $K_2(x)$ used to begin the iteration are taken as 3.0.

The inverse solutions using the inexact measurements are shown in Figures (4.5) and (4.6).

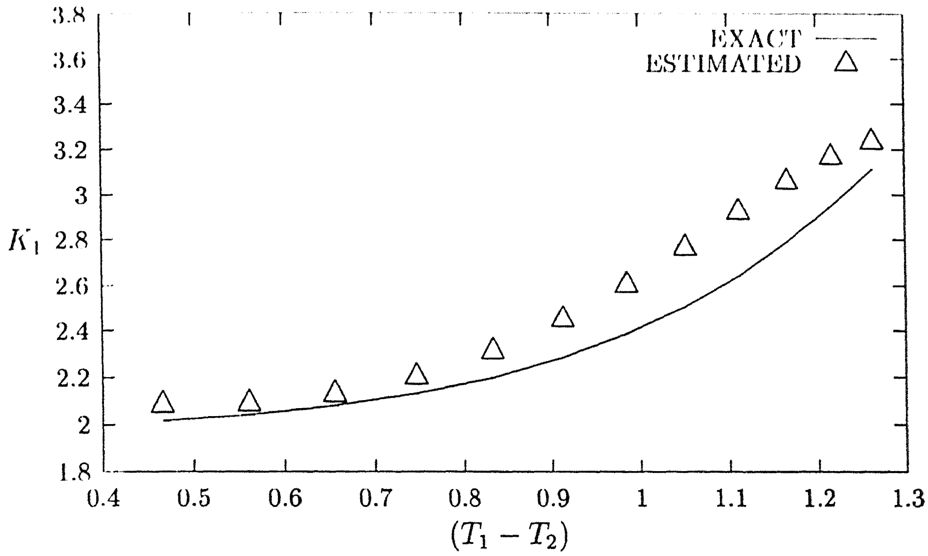

Figure 4.3: Estimated function of $K_1(T_1 - T2)$ with $\sigma = 0.0$

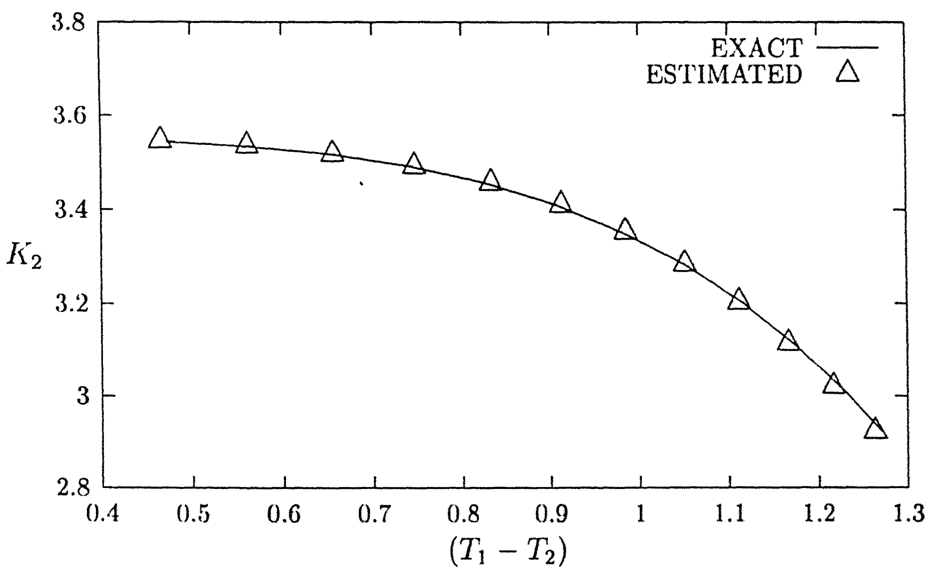

Figure 4.4: Estimated function of $K_2(T_1 - T2)$ with $\sigma = 0.0$

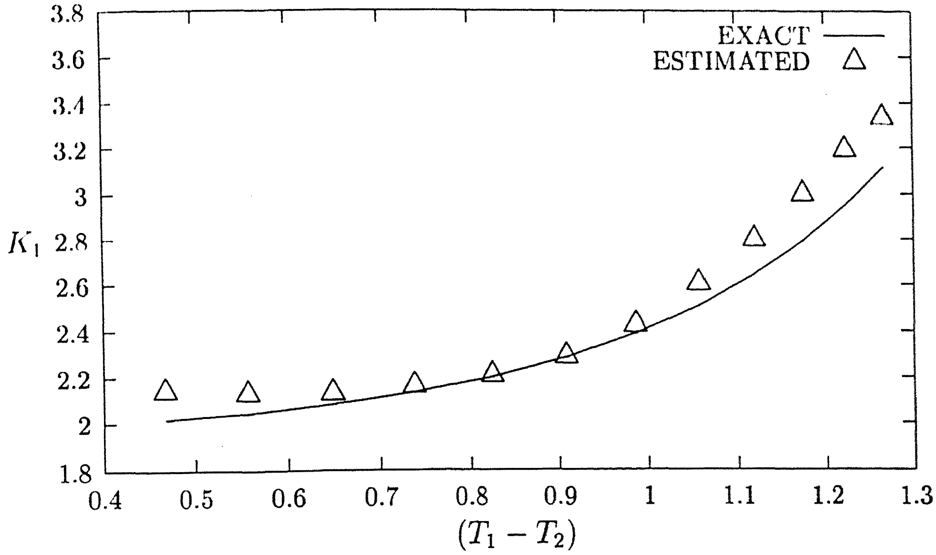

Figure 4.5: Estimated function of $K_1(T_1 - T2)$ with $\sigma = 0.001$

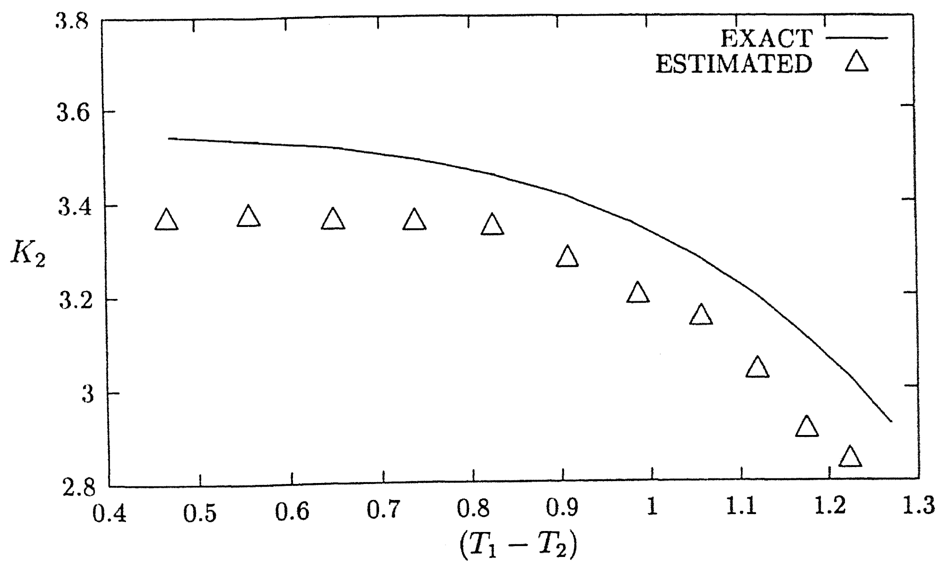

Figure 4.6: Estimated function of $K_2(T_1 - T2)$ with $\sigma = 0.001$

2.2 Transient Problem

methodology for simultaneously determining unknown parameters $K_1(T_1, T_2)$, $K_2(T_1, T_2)$ $C(T_1, T_2)$ has been described in Section 2.4.2.

arameter Sensitivity

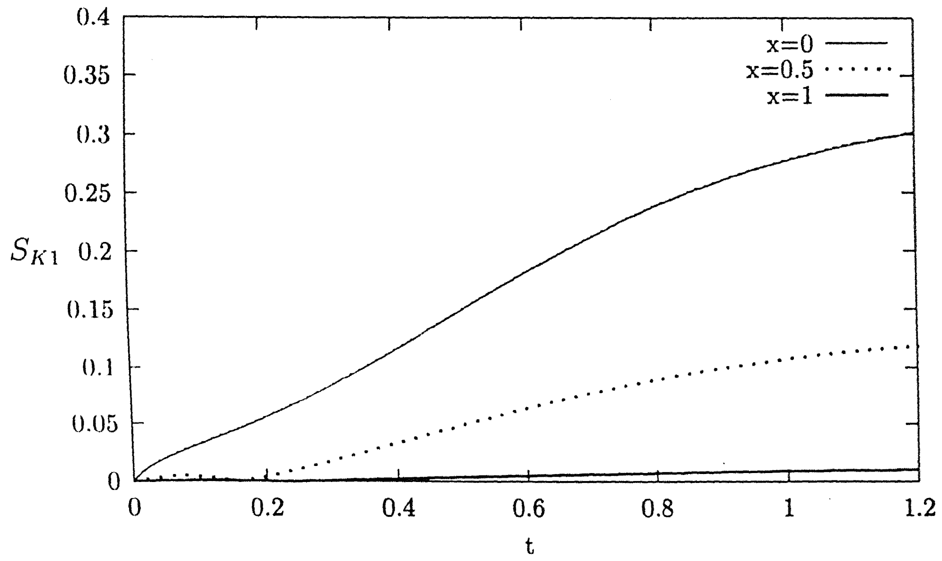

Figure 4.7: Variation of sensitivity coefficient of K_1 as a function of time

Figures (4.7-4.9) show the variation of the sensitivity coefficients for K_1, K_2 and C unction of time. The sensitivity coefficients S_{K1}, S_{K2} and S_C are defined as:

$$S_{K1} = \left|\frac{(\Delta T_1)_{K1} - (\Delta T_2)_{K1}}{\Delta K_1}\right| \tag{4.5}$$

$$S_{K2} = \left|\frac{(\Delta T_1)_{K2} - (\Delta T_2)_{K2}}{\Delta K_2}\right| \tag{4.6}$$

$$S_C = \left|\frac{(\Delta T_1)_C - (\Delta T_2)_C}{\Delta C}\right| \tag{4.7}$$

res (4.7-4.9) show that the sensitivity coefficients for K_1, K_2 and C are very small at 1 and a maximum at $x = 0$. The figures also indicates that sensitivities for K_2 and C

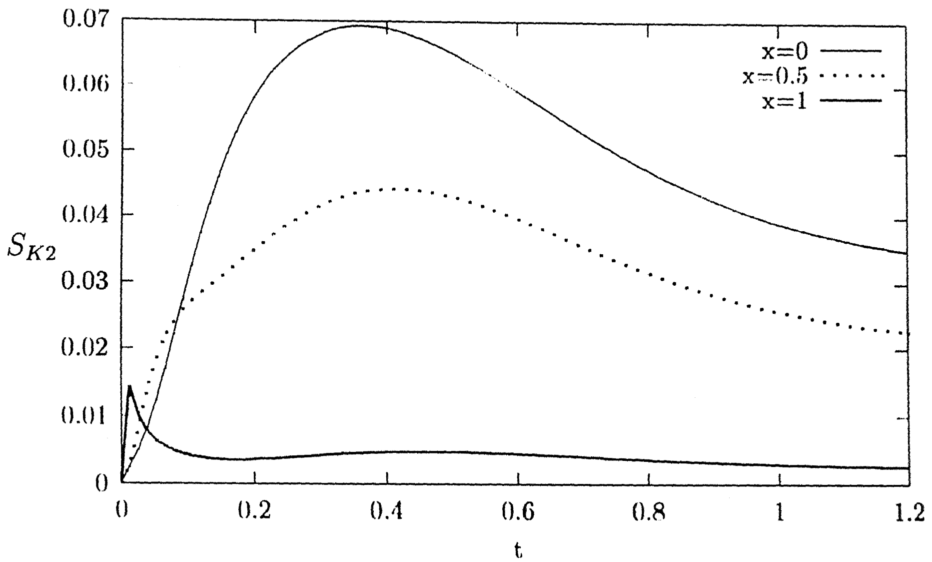

Figure 4.8: Variation of sensitivity coefficient of K_2 as a function of time

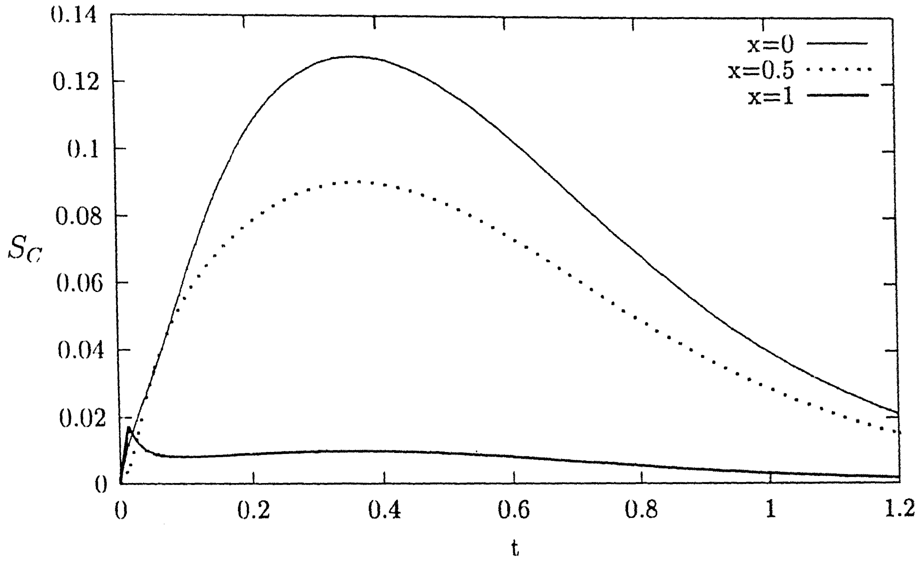

Figure 4.9: Variation of sensitivity coefficient of C as a function of time

are maximum at around $t = 0.4$. On the other hand, the sensitivity for K_1 is maximum at $t = t_f$. The above results provide very important information about the solutions of the inverse problem. The estimated values of K_2 and C are expected to be close to the actual values at the points close to $x = 0$ and $t = 0.4$. Similarly, the estimated values of K_1 will be more accurate for a time close to $t = t_f$. From the adjoint Equation (2.295) we see that the adjoint functions are zero at the final time step. Therefore, the estimated solutions of K_2 and C will deviate from the actual values near final time step. Figures (4.7-4.9) also show that the sensitivity curves of parameter K_2 are flatter compared to the other two parameters.

Solution of the Inverse Problem

To illustrate the validity of the conjugate gradient method in simultaneously predicting $K_1(T_1, T_2)$, $K_2(T_1, T_2)$ and $C(T_1, T_2)$ we consider an example. Here the exact functional form of K_1, K_2 and C are taken to be second-order polynomials with $(T_1 - T_2)$ as the dependent variable, i.e.

$$K_1(T_1, T_2) = a_0 + a_1 \times (T_1 - T_2) + a_2 \times (T_1 - T_2)^2 \tag{4.8}$$

$$K_2(T_1, T_2) = b_0 + b_1 \times (T_1 - T_2) + b_2 \times (T_1 - T_2)^2 \tag{4.9}$$

$$C(T_1, T_2) = c_0 + c_1 \times (T_1 - T_2) + c_2 \times (T_1 - T_2)^2 \tag{4.10}$$

where the constants a_0, a_1 and a_2 for $K_1(T_1, T_2)$ are taken as 5.0, -1.5 and -0.5 respectively, the constants b_0, b_1 and b_2 for $K_2(T_1, T_2)$ are taken as 4.5, 1.5 and 1.0 respectively, and the constants c_0, c_1 and c_2 for C are chosen as 3.5, -1.5 and -1.0 respectively. The initial values of both the state variables T_1 and T_2 are taken as 1.0. The boundary at $x = 0$ is subjected to constant fluxes q_1 and q_2, while at $x = 1$, T_1 and T_2 are kept constant at T_{1l} and T_{2l} respectively. In all the test cases considered hare, the values of q_1 and q_2 are taken as 5.0, 1.0 respectively. The values of both T_{1l} and T_{2l} are assumed to be 1.0.·

The space and time increments are taken as $\Delta x = 0.02$ and $\Delta t = 0.02$ respectively in the finite difference calculations. The total measurement time is chosen as $t_f = 1.2$. The measurement spacing Dx is assumed to be same as finite difference spacing Δx and the measurement time step Dt is taken the same as Δt of the direct problem.

From the numerical experiments it has been observed that the inverse solutions of the problem depend on the initial guesses. This is because three unknown functions, $K_1(x,t)$, $K_2(x,t)$ and $C(x,t)$, are to be estimated simultaneously by using only the measured values $Y_1(x,t)$ and $Y_2(x,t)$. This requires that the estimated values $T_1(x,t)$ and $T_2(x,t)$ obtained by utilizing any combination of $K_1(x,t)$, $K_2(x,t)$ and $C(x,t)$ could possibly be equal to $Y_1(x,t)$ and $Y_2(x,t)$ respectively. But the estimated properties are not necessarily correct. That is why the initial guesses cannot be chosen arbitrarily. The initial guesses should be taken to be close to average values of the parameters. If the initial guesses are far from the the actual values, the inverse solutions deviate from the actual solutions. In all the test cases considered here, initial guesses of $K_1(x,t)$, $K_2(x,t)$ and $C(x,t)$ used to begin the iteration are taken as 5.0, 4.2 and 3.2 respectively.

The estimated functions of $K_1(x,t)$, $K_2(x,t)$ and $C(x,t)$, obtained by using the exact measurement data, $\sigma = 0.0$, are shown in Figures (4.10, 4.12 and 4.14) respectively.

In order to compare the results for situations involving random measurement errors, normally distributed uncorrelated errors with zero mean and constant standard deviation are superimposed on the measurement data. The simulated inexact measurement data Y_1 and Y_2 are given by Equations (4.3) and (4.4). In this calculation, it is assumed that the standard deviations for both the measured values Y_1 and Y_2 are the same. The dimensionless measured values of Y_1 and Y_2 with errors $\sigma = 0.001$ are obtained according to Equation (4.3) and (4.4). The inverse solutions using these inexact measurements are shown in Figures (4.11, 4.13 and 4.15). The figures show the estimated values of the parameters at $x = 0.25$. The estimated values of the parameters K_1, K_2 and C have been determined in the time interval of $t = 0.2$ and $t = 0.4$ since the corresponding errors were found to be a minimum. The comparison among the figures show that the estimated values of K_1 are more accurate as compared to K_2 and C. These results also agree with the sensitivity analysis.

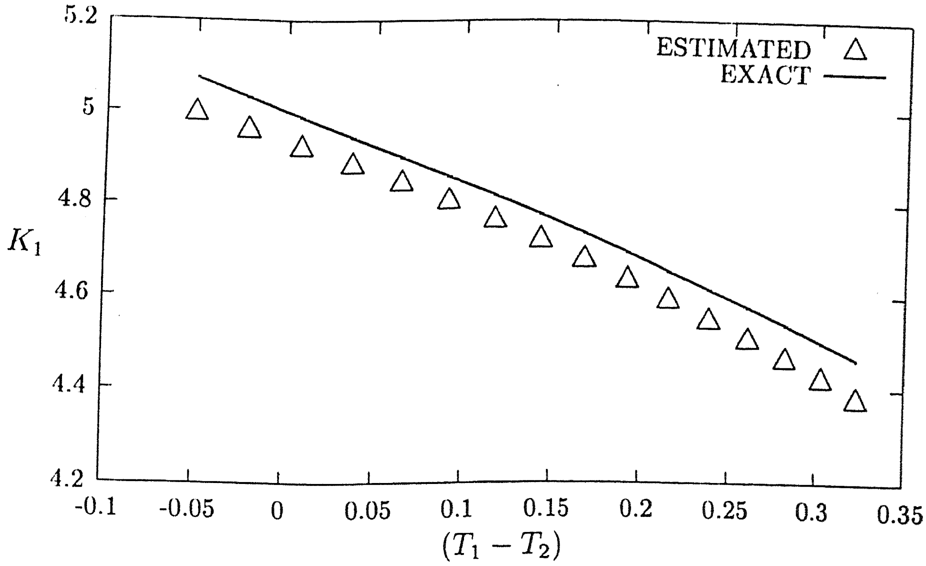

Figure 4.10: Exact and estimated values of K_1 at $x = 0.25$ with $\sigma = 0$

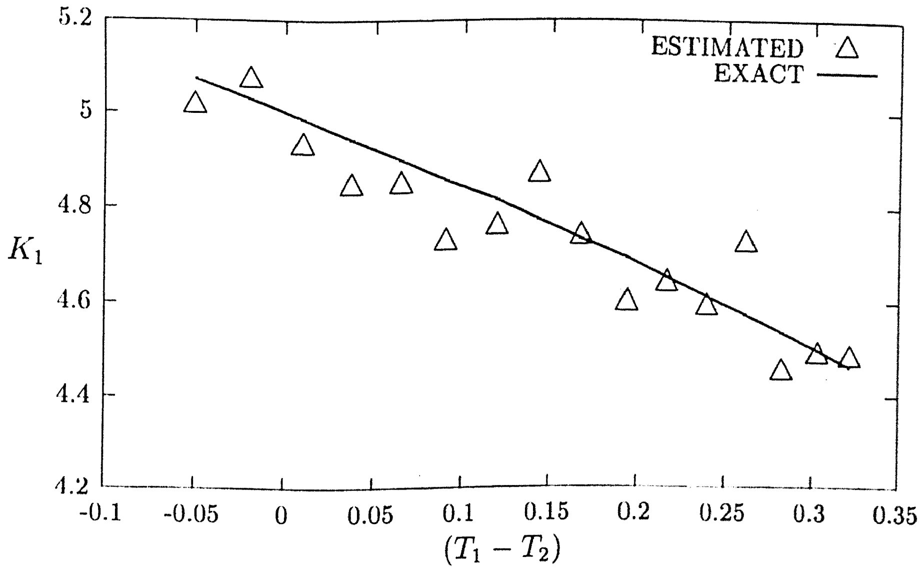

Figure 4.11: Exact and estimated values of K_1 at $x = 0.25$ with $\sigma = 0.001$

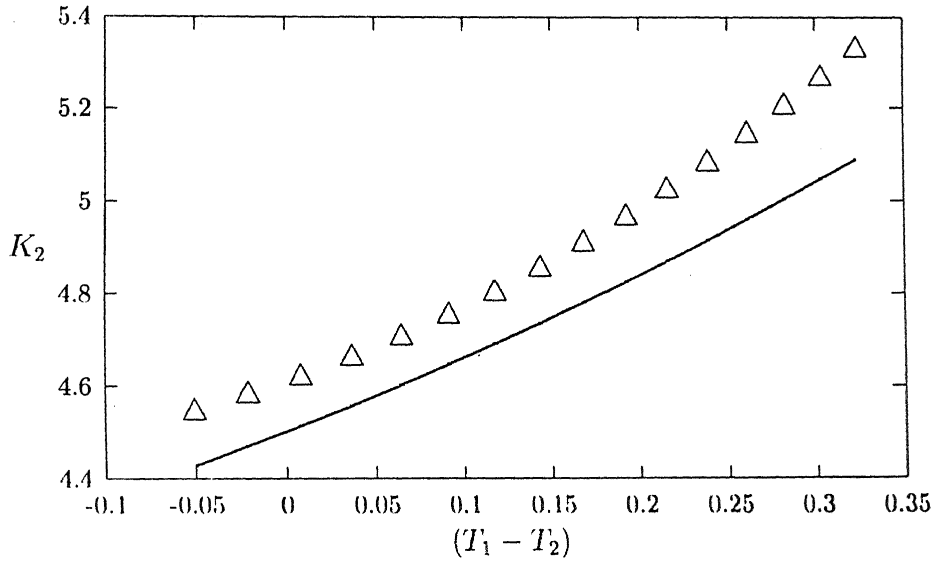

Figure 4.12: Exact and estimated values of K_2 at $x = 0.25$ with $\sigma = 0$

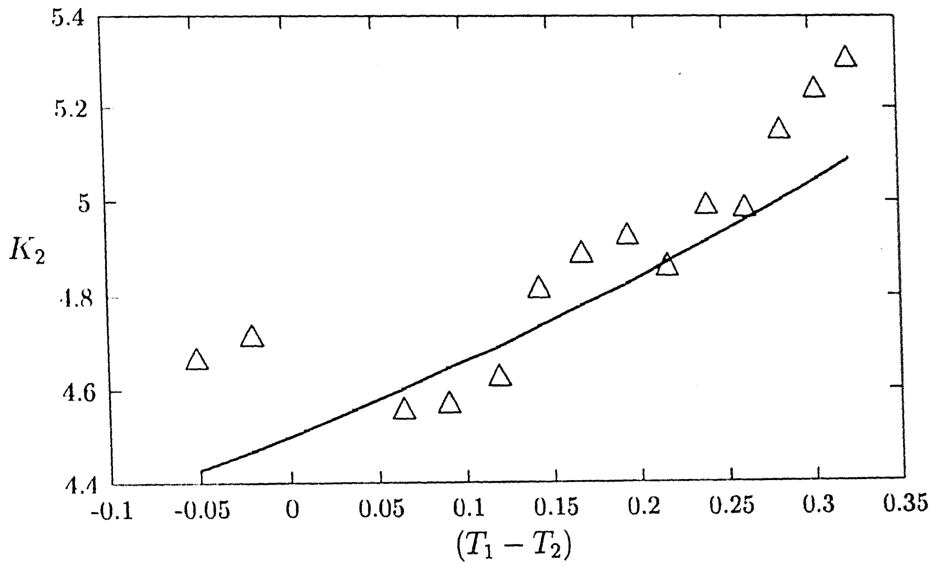

Figure 4.13: Exact and estimated values of K_2 at $x = 0.25$ with $\sigma = 0.001$

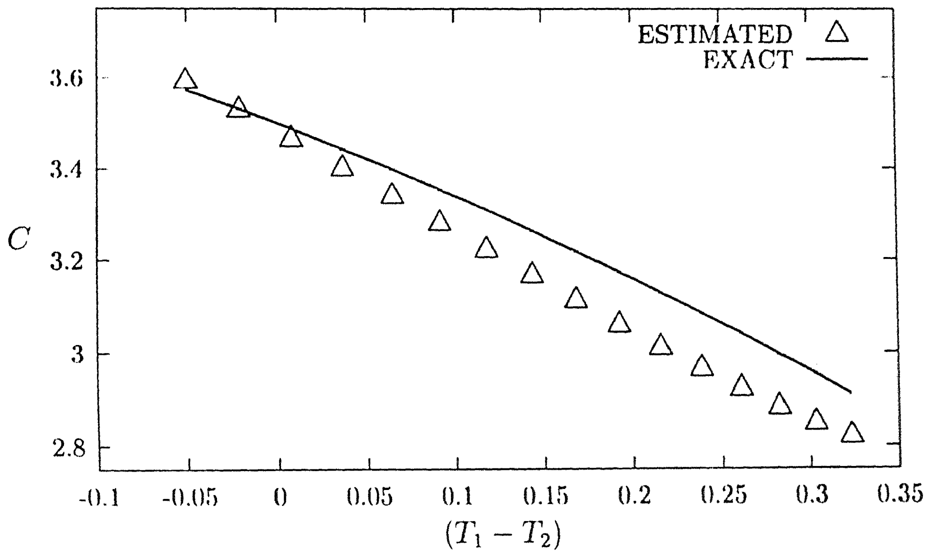

Figure 4.14: Exact and estimated values of C at $x = 0.25$ with $\sigma = 0$

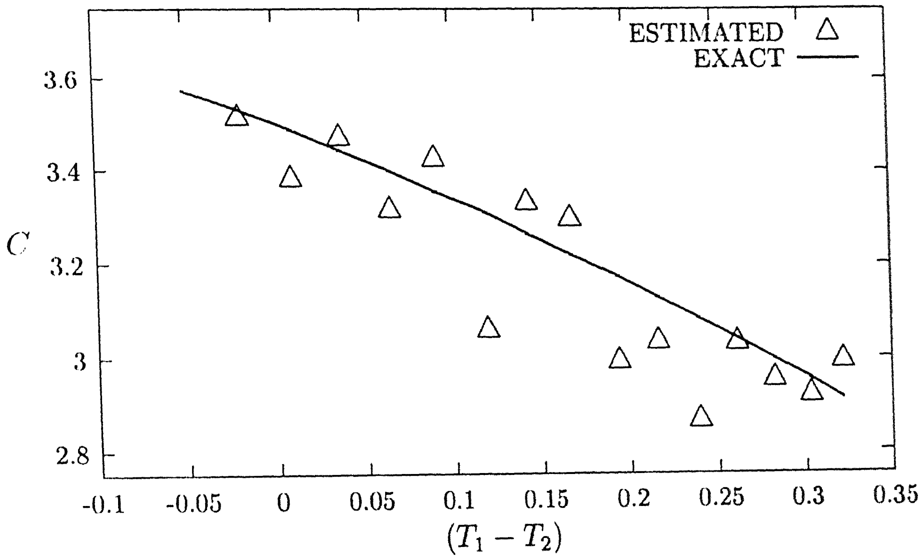

Figure 4.15: Exact and estimated values of C at $x = 0.25$ with $\sigma = 0.001$

4.3 Estimation of Parameters for Coupled Equations with Source Term

The mathematical formulations of the problem has been stated in Section 2.5.

Sensitivity Analysis

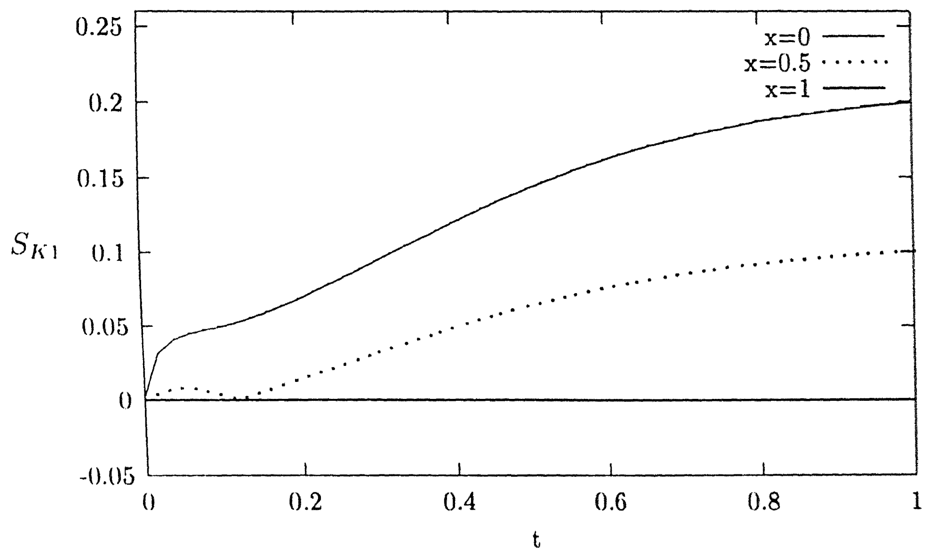

Figure 4.16: Variation of Sensitivity Coefficients of K_1 as a function time

Figures (4.16-4.18) show the distribution of sensitivity coefficients for K_1, K_2 and C at $x = 0.0$, 0.5 and 1.0. The sensitivity coefficients S_{K1}, S_{K2} and S_C are given by Equations (4.6), (4.7) and (4.7) respectively. The figures show that the sensitivity coefficients are the highest at $x = 0$ as compared to other locations. The sensitivities of the parameters decrease with x and finally go to zero at $x = 1$. It is observed that the sensitivity of K_1 at any point x is a maximum at t_f. The sensitivity of K_2 is maximum for a time close to $t = t_f$. The sensitivity C at any point x is observed to be maximum at a time between $t = 0.2$ and 0.4. The above observations indicate that the information obtained from the inverse analysis about the parameter K_1 is the best for the points close to $x = 0$ and for time close to final time, t_f. From the adjoint Equations (2.295) it is clear that the adjoint functions, λ_1 and λ_2 are zero at $t = t_f$ Therefore, the inverse analysis does not give satisfactory results for the final time step. The above sensitivity analysis

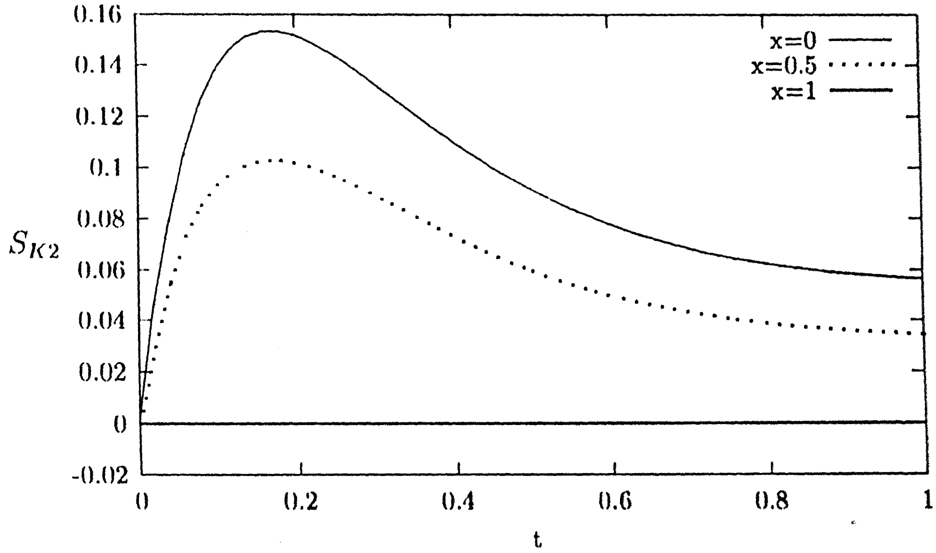

Figure 4.17: Variation of Sensitivity Coefficients of K_2 as a function time

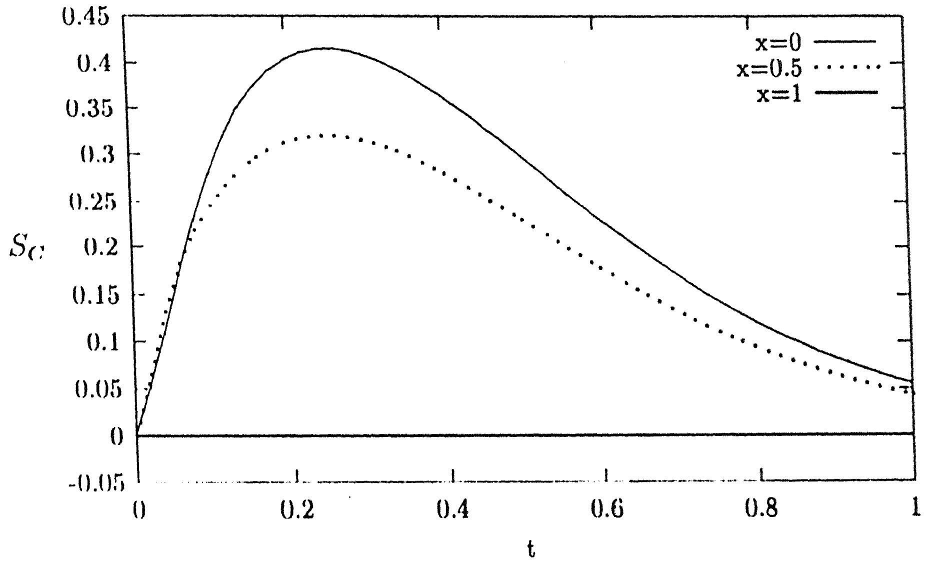

Figure 4.18: Variation of Sensitivity Coefficients of C as a function time

indicates that the estimated values of K_2 are more accurate at points close to $x = 0$ and a time close to $t = 0.2$. The estimated values of C are expected to be satisfactory at the points close to $x = 0$ for time between $t = 0.2$ and 0.4.

Solution of the Inverse Problem

To illustrate the validity of the above statements, we consider a specific example where the exact functional form of K_1 and K_2 are assumed to be third-order polynomials while C is taken as a second-order polynomial with $(T_1 - T_2)$ as the dependent variable. Hence

$$K_1(T_1, T_2) = a_0 + a_1 \times (T_1 - T_2) + a_2 \times (T_1 - T_2)^2 + a_3 \times (T_1 - T_2)^3 \quad (4.11)$$

$$K_2(T_1, T_2) = b_0 + b_1 \times (T_1 - T_2) + b_2 \times (T_1 - T_2)^2 + b_3 \times (T_1 - T_2)^3 \quad (4.12)$$

$$C(T_1, T_2) = c_0 + c_1 \times (T_1 - T_2) + c_2 \times (T_1 - T_2)^2 \quad (4.13)$$

where the constants a_0, a_1, a_2 and a_3 for $K_1(T_1, T_2)$ are taken as 5.5, -1.0, -0.5 and -0.1 respectively, the constants b_0, b_1, b_2 and b_3 for $K_2(T_1, T_2)$ are taken as 5.5, 1.5, 1.0 and 0.5 respectively, and the constants c_0, c_1 and c_2 are chosen as 1.5, -0.75 and -0.2 respectively. The initial values of the variables T_1 and T_2 are taken as 1.0 and 2.0 respectively. The boundary at $x = 0$ is subjected to constant fluxes $q_1 = 6.0$ and $q_2 = 2.0$. The state variables T_1 and T_2 are kept at the constant values of T_{1l} and T_{2l} respectively, at the other boundary at $x = 1$. Both the values of T_{1l} and T_{2l} are taken as 1.0.

The space and time increments are taken as $\Delta x = 0.05$ and $\Delta t = 0.02$ respectively, in the finite difference calculations. The total measurement time is chosen as $t_f = 1.0$. The measurement spacing Dx is assumed to be same as the finite difference spacing Δx and the measurement time step Dt is taken as the same as finite difference time step Δt. The estimated functions of $K_1(x,t)$, $K_2(x,t)$ and $C(x,t)$ obtained with measurement errors $\sigma = 0.0$ and $\sigma = 0.005$ are shown in Figures (4.19-4.24). Figures (4.19), (4.21) and (4.23) show the estimated values of the parameters K_1, K_2 and C respectively at $x = 0.25$ for time between 0.15 and 0.5. The estimated values of the parameters at $x = 0.5$ for the same time range are shown in Figures (4.20), (4.22) and (4.24).

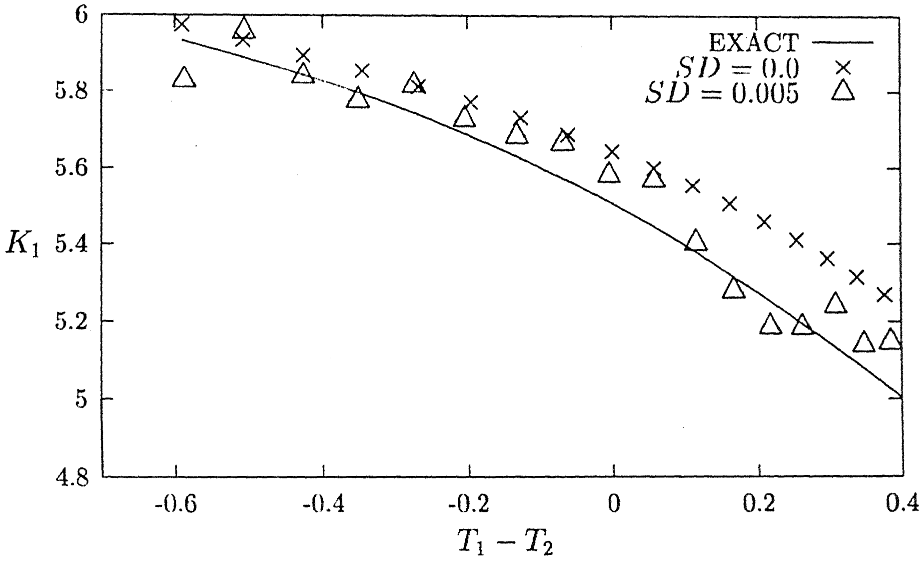

Figure 4.19: Exact and estimated values of $K_1(T_1 - T_2)$ at $x = 0.25$

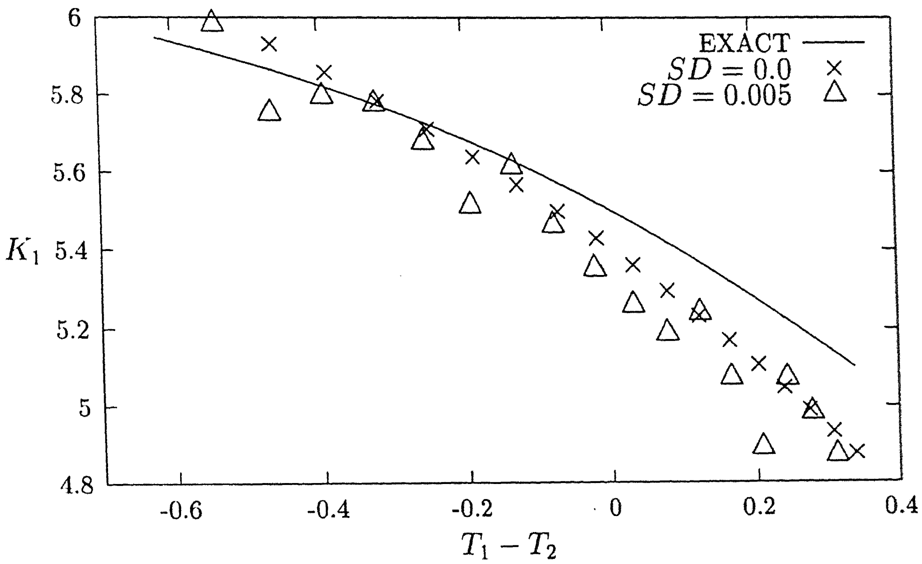

Figure 4.20: Exact and estimated values of $K_1(T_1 - T_2)$ at $x = 0.50$

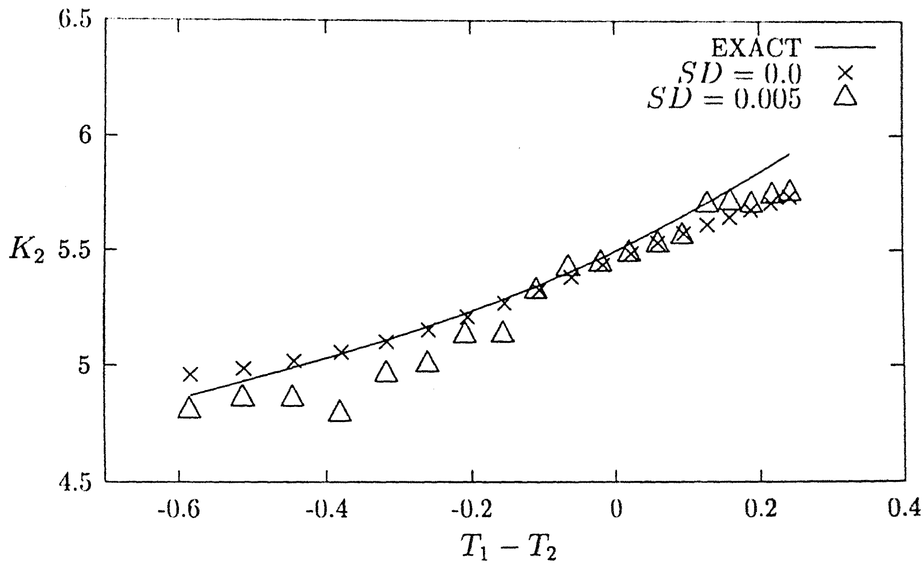

Figure 4.21: Exact and estimated values of $K_2(T_1 - T_2)$ at $x = 0.25$

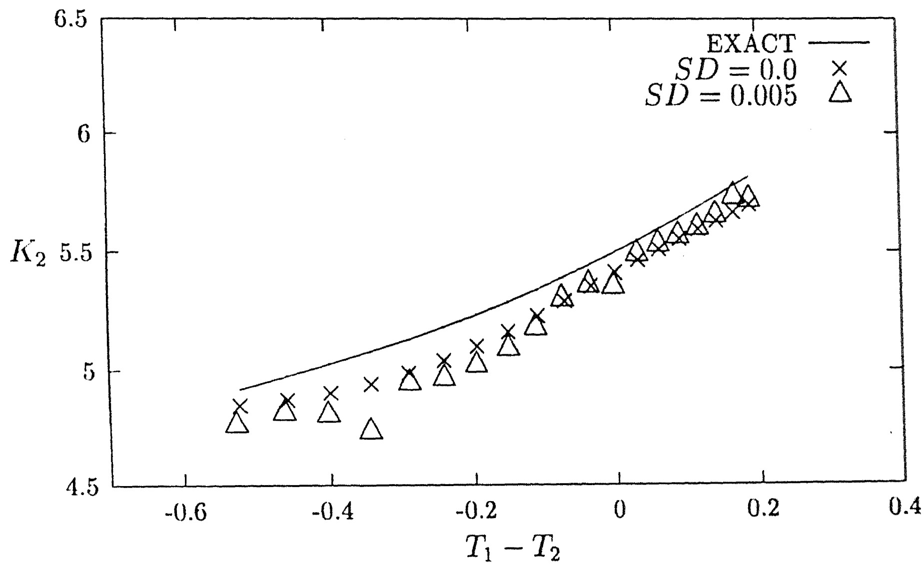

Figure 4.22: Exact and estimated values of $K_2(T_1 - T_2)$ at $x = 0.50$

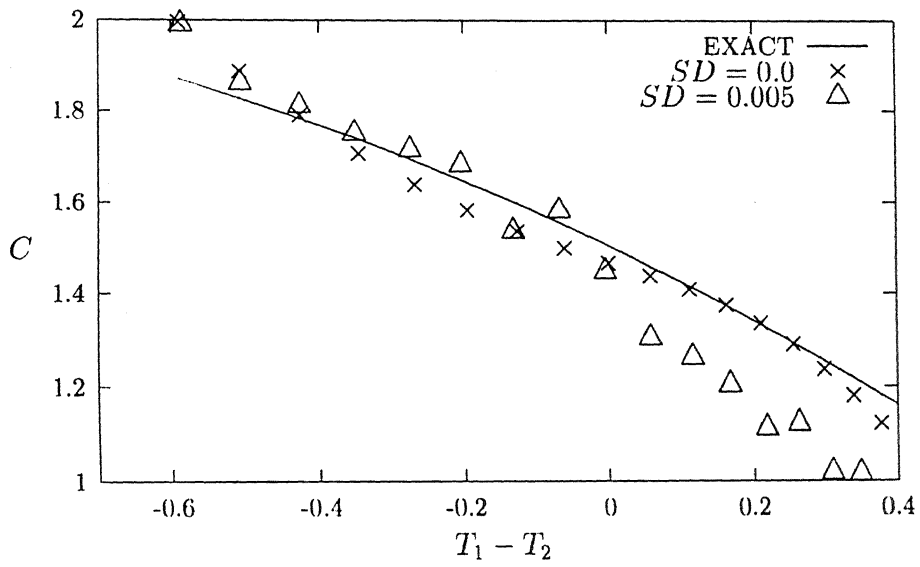

Figure 4.23: Exact and estimated values of $C(T_1 - T_2)$ at $x = 0.25$

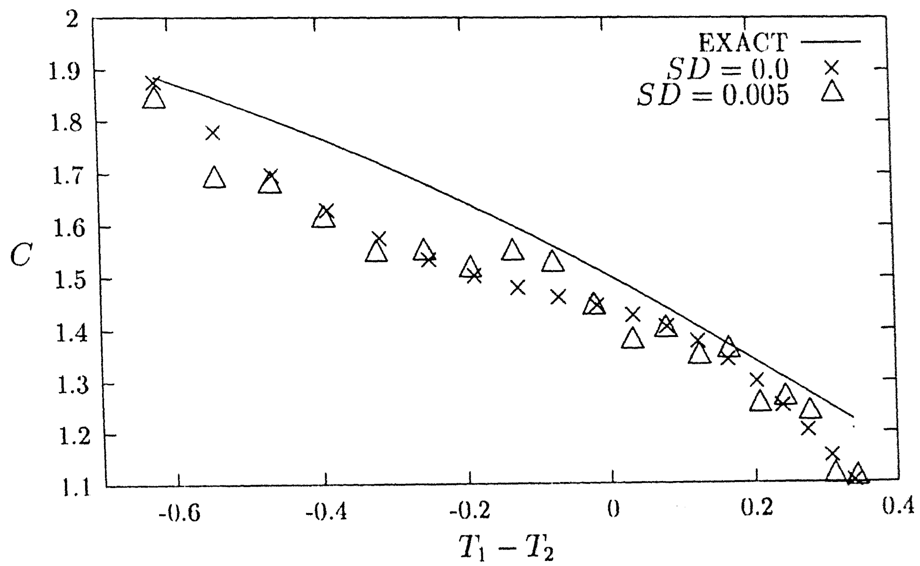

Figure 4.24: Exact and estimated values of $C(T_1 - T_2)$ at $x = 0.50$

Table 4.1: The convergence parameters for coupled steady state problem

Measurement error, σ	Stop Criterion $\lvert J^{n+1} - J^n \rvert$	Number of iterations	CPU time (s)	$(K_1)_{rms}$	$(K_2)_{rms}$
0.000	10^{-5}	20	0.16	0.166	0.090
0.001		20	0.36	0.165	0.159

Table 4.2: The convergence parameters for coupled inverse problem without source term

Measurement error, σ	Stop Criterion $\lvert J^{n+1} - J^n \rvert$	Number of iterations	CPU time (s)	$(K_1)_{rms}$	$(K_2)_{rms}$	C_{rs}
0.000	10^{-7}	142	30.83	0.267	0.58	1.15
0.001		128	28.24	0.25	0.59	1.07

Table 4.3: The convergence parameters for coupled inverse problem with source term

Measurement error, σ	Stop Criterion $\lvert J^{n+1} - J^n \rvert$	Number of iterations	CPU time (s)	$(K_1)_{rms}$	$(K_2)_{rms}$	C_{rms}
0.000	10^{-5}	27	21.53	0.385	0.568	0.251
0.001		28	21.55	0.384	0.555	0.332

Chapter 5

Oil-Water Flow in an Unsaturated Porous Medium

5.1 Introduction

There are some important property relationships to be reconstructed in reservoir engineering calculations. Consider oil-water flow in a porous formation, for example. These properties include relative permeability of oil, relative permeability of water, capillary pressure, porosity of the medium, fluid density, specific heat and thermal conductivity of the fluid-saturated rock, viscosity of water and petroleum fluids, enthalpy and specific heat for water and petroleum fluids.

It has been observed that the relative permeability of oil and water and capillary pressure depend on water and oil saturation. For homogeneous medium, porosity remains constant. The porosity of consolidated rocks (encountered in oil reservoirs) depends on the packing of the grains, their shape, arrangement and size distribution. It is obvious that the porosity of such medium may vary from point to point. Density of petroleum liquids depend on temperature as well. The specific heat and thermal conductivity of fluid saturated rock also vary with temperature. The viscosity of oil and water also depend on temperature.

All the above constitutive relationships are extremely important during the simulation of oil recovery. These parameters are generally not measurable from the physical point-of-view. The inverse approach provides a way whereby measurements of state are

used to determine the unknown parameters by fitting the model output with the measurements.

The present chapter addresses the development of the coupled inverse analysis for estimating simultaneously the three parameters, relative permeability of oil, relative permeability of water and capillary pressure, as are encountered in oil-water flow in a porous medium. The flow is considered to be isothermal. Also the fluids are assumed to be incompressible.

The mathematical formulation of the inverse problem is given in Section 2.6.

5.2 Results and Discussions

The mathematical model of oil-water flow in a porous medium leads the problem of coupled equations with Source terms as discussed in Section 4.3. Therefore, the analysis of the sensitivity coefficients for K_o, K_w and C are similar to the sensitivity coefficients for K_1, K_2 and C respectively. The parameters K_o, K_w and C are given by Equation (2.322). The exact functional form of the parameters K_o and K_w are assumed to be third-order polynomials of non-dimensional capillary pressure, P_c. The parameter C is taken as a second-order polynomial with P_c as the dependent variable. The exact functional form of these parameters are expressed as

$$K_O(P_c) = a_0 + a_1 P_c + a_2 P_c^2 + a_3 P_c^3 \tag{5.1}$$

$$K_w(P_c) = b_0 + b_1 P_c + b_2 P_c^2 + b_3 P_c^3 \tag{5.2}$$

$$C(P_c) = c_0 + c_1 P_c + c_2 P_c^2 \tag{5.3}$$

where the constants a_0, a_1, a_2 and a_3 are taken as 3.2, 1.5, -1.5, and -0.45 respectively, the constants b_0, b_1, b_2 and b_3 are taken as 3.0, -1.25, 1.25 and 0.4 respectively, and the constants c_0, c_1, c_2 are chosen as 2.0, 1.5 and -0.15, respectively. Oil and water pressure is assumed to be constant and equal to 1.0 at $t = 0$. One boundary is subjected to constant fluxes $q_o = 1$ and $q_w = 1$ while the other boundary is kept at constant pressures $P_o = 1.5$ and $P_w = 1.0$.

The space and time increments are taken as 0.05 and 0.02 respectively in the finite difference calculations. The estimated functions K_o, K_w and C, obtained by using measurement data with $\sigma = 0.0$, $\sigma = 0.005$ are shown in Figures (5.1-5.6). The estimated

parameters are shown for two locations, namely $x = 0.2$ and $x = 0.4$. In all the cases, the initial guesses of K_o, K_w and C are taken as 2.5, 3.0 and 1.5 respectively.

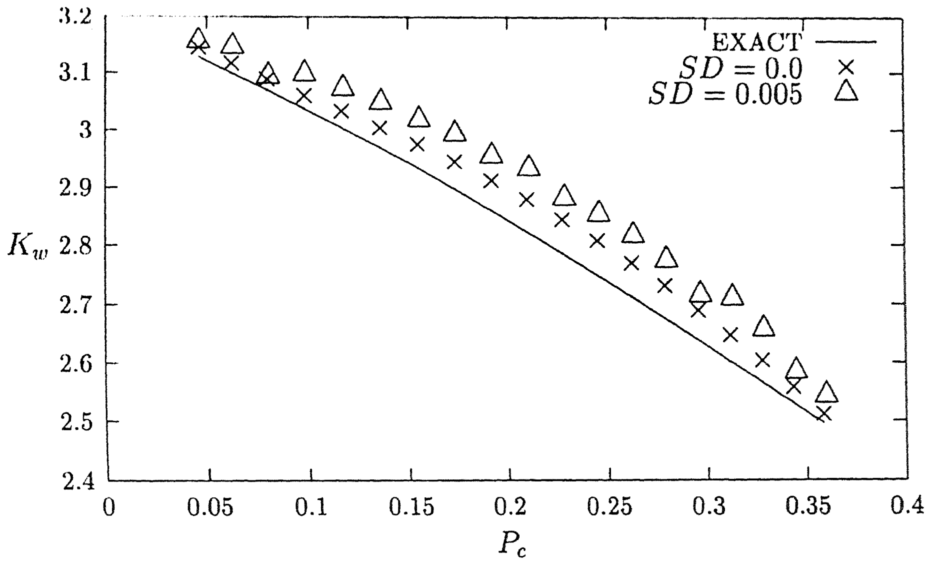

Figure 5.1: Exact and estimated values of $K_w(P_c)$ at $x = 0.2$

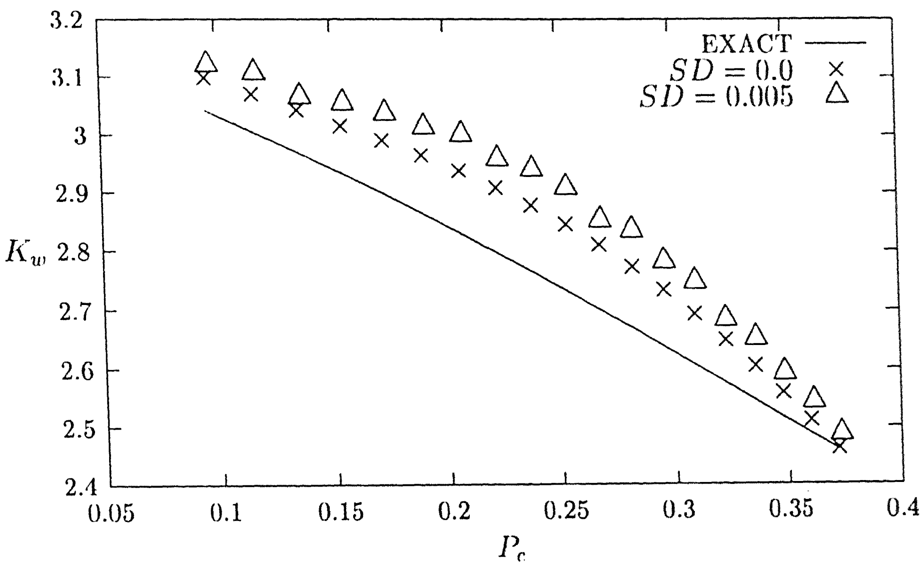

Figure 5.2: Exact and estimated values of $K_w(P_c)$ at $x = 0.4$

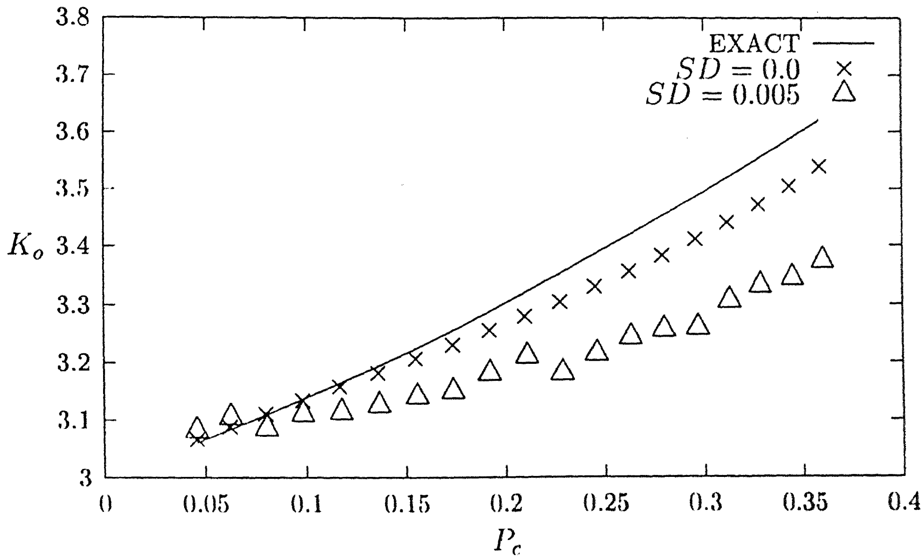

Figure 5.3: Exact and estimated values of $K_o(P_c)$ at $x = 0.2$

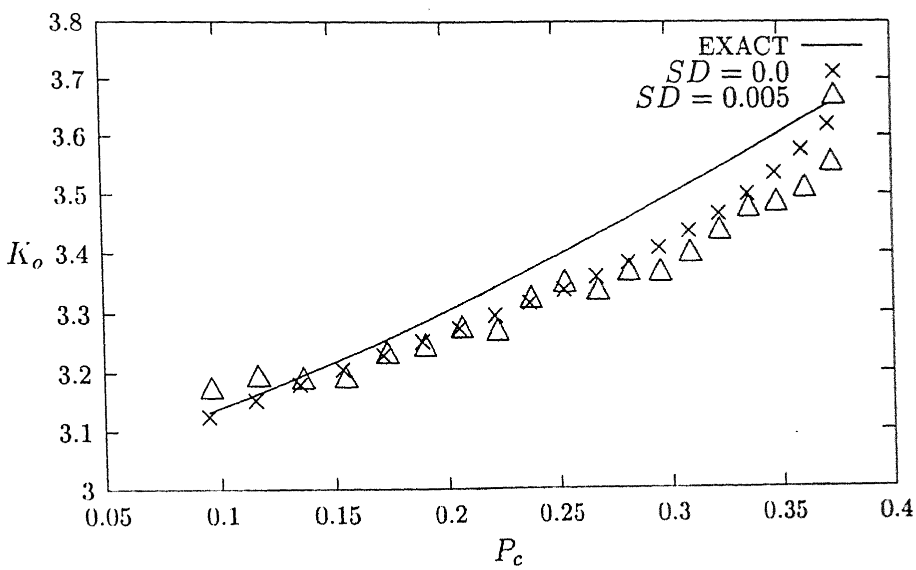

Figure 5.4: Exact and estimated values of $K_o(P_c)$ at $x = 0.4$

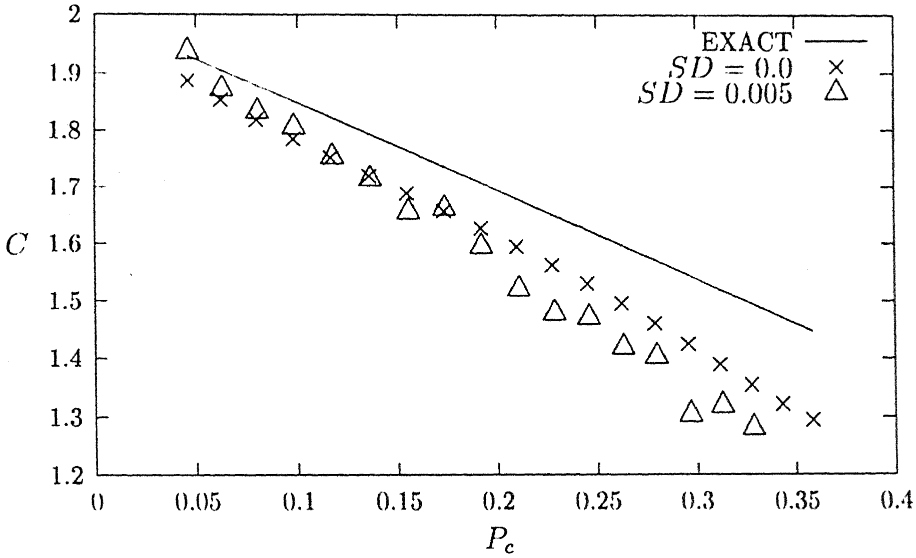

Figure 5.5: Exact and estimated values of $C(P_c)$ at $x = 0.2$

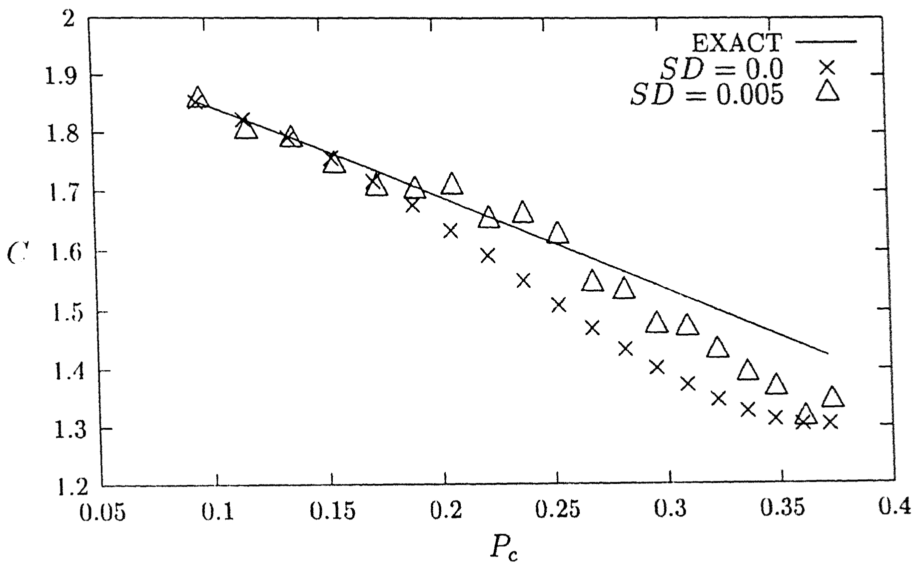

Figure 5.6: Exact and estimated values of $C(P_c)$ at $x = 0.4$

Chapter 6

Conclusions and Scope for Future Work

6.1 Conclusions

Details of an inverse technique for a one dimensional nonlinear diffusion problem employing the conjugate gradient method have been discussed in the present study. The conjugate gradient method provides an efficient, rapidly convergent and a systematic approach for the solution of the inverse heat conduction and the coupled inverse problem. Numerical results show that the conjugate gradient method does not require *a priori* information on the functional form of the parameters to be estimated. Sensitivity analyses required during the inverse procedure is seen to be a useful tool for designing an experiment.

The following conclusions have been drawn in the present study:

Heat Conduction

1. Parameter estimation is exact if K and C are constants and in pure steady state problems.
2. In general, reconstruction is qualitatively acceptable.
3. Errors increase with the measurement error, σ.

4. Larger errors are seen near regions of small temperature gradients and the specified temperature boundary. Excessive dependence on the steady state data in an unsteady formulation is also seen to contribute to large errors.

Coupled Diffusion Problem

1. Reconstruction of the parametric functions is qualitatively acceptable.
2. Errors increase with the measurement error, σ. Errors are generally higher than in the single equation model. The convergence rates are sensitive to the initial guesses. It is best to prescribe average values of the parameters at the start of the calculation.
3. Larger errors are seen near regions of small gradients of the dependent variables and boundaries with Dirichlet boundary conditions.
4. The inverse procedure is seen to be applicable for determining constitutive relations in oil-water flow in a porous medium.

6.2 Scope for Future Work

6.2.1 Experiments

In all cases considered in the study the input data is taken from numerical results. The errors are assumed to be random. In practice, the experimental errors are different. Therefore, are needs to estimate the parameters with real experimental data.

6.2.2 Advection-diffusion Problems

The inverse procedure should be extended to equations of the type

$$C\left[\frac{\partial T}{\partial t} + u.\nabla T\right] = \nabla(K(T)\nabla T) + Q$$

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Appendix A

A.1 Discretization of the Direct Problem

Consider the following direct problem wherein the method of discretization of a nonlinear equation is presented:

$$\frac{\partial}{\partial x}\left(K(T)\frac{\partial T(x,t)}{\partial x}\right) = C(T)\frac{\partial T(x,t)}{\partial t} \tag{A.1}$$

Integrating the above equation over a control volume around the i th node and at $n+1$ th time level (Figure A.1), we obtain

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left[\frac{\partial}{\partial x}\left(K(T)\frac{\partial T(x,t)}{\partial x}\right)\right]^{n+1} dx = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left[C(T)\frac{\partial T(x,t)}{\partial t}\right]^{n+1} dx$$

$$\text{Or} \quad \left[K^{n+1}\frac{\partial T^{n+1}(x,t)}{\partial x}\right]_{i+\frac{1}{2}} - \left[K^{n+1}\frac{\partial T^{n+1}(x,t)}{\partial x}\right]_{i-\frac{1}{2}} = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left[C\frac{\partial T(x,t)}{\partial t}\right]^{n+1} dx$$

$$\text{Or} \quad K^{n+1}_{i+\frac{1}{2}}\frac{T^{n+1}_{i+1} - T^{n+1}_{i}}{\Delta x} - K^{n+1}_{i-\frac{1}{2}}\frac{T^{n+1}_{i} - T^{n+1}_{i-1}}{\Delta x} = C^{n+1}_{i}\frac{T^{n+1}_{i} - T^{n}_{i}}{\Delta t}\Delta x$$

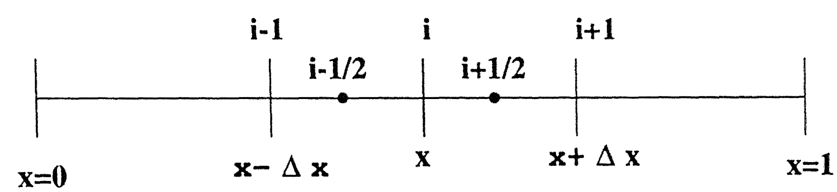

Figure A.1: Control Volume Formulation

$$\text{Or}\quad \left(\frac{K_{i+1}^{n+1}+K_i^{n+1}}{2}\right)\frac{T_{i+1}^{n+1}-T_i^{n+1}}{\Delta x} - \left(\frac{K_i^{n+1}+K_{i-1}^{n+1}}{2}\right)\frac{T_i^{n+1}-T_{i-1}^{n+1}}{\Delta x}$$
$$= C_i^{n+1}\frac{T_i^{n+1}-T_i^n}{\Delta t}\,\Delta x$$

$$\text{Or}\quad -\left(K_{i+1}^{n+1}+K_i^{n+1}\right)T_{i+1}^{n+1} + \left[\left(K_{i+1}^{n+1}+2K_i^{n+1}+K_{i-1}^{n+1}\right)+2\frac{C_i^{n+1}(\Delta x)^2}{\Delta t}\right]T_i^{n+1}$$
$$-\left(K_i^{n+1}+K_{i-1}^{n+1}\right)T_{i-1}^{n+1} = 2\frac{C_i^{n+1}(\Delta x)^2}{\Delta t}\,T_i^n \qquad \text{(A.2)}$$

where the n th level is a known, state and the $n+1$ th time level is assumed to be unknown.

A.2 Discretization of the Adjoint Problem and the Treatment of the Dirac-Delta Function

Consider the adjoint problem given by the Equation (2.79):

$$\frac{\partial}{\partial x}\left(K(x,t)\frac{\partial\lambda}{\partial x}\right)+\frac{\partial(C\lambda)}{\partial t}+2\sum_{i=2}^{M-1}[T-Y]\delta(x-x_i)=0 \qquad \text{(A.3)}$$

Integrating the above equation over a control volume around the i th node and at $n-1$ th time level, we obtain

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\left[\frac{\partial}{\partial x}\left(K\frac{\partial\lambda}{\partial x}\right)\right]^{n-1}dx+\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\left[\frac{\partial(C\,\lambda)}{\partial t}\right]^{n-1}dx+\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}2\sum_{i=2}^{M-1}[T^{n-1}-Y^{n-1}]\delta(x-x_i)\,dx=0$$

$$\text{Or}\quad \left[K^{n-1}\frac{\partial\lambda^{n-1}}{\partial x}\right]_{i+\frac{1}{2}} - \left[K^{n-1}\frac{\partial\lambda^{n-1}}{\partial x}\right]_{i-\frac{1}{2}}$$
$$+\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\left[\frac{\partial C\lambda}{\partial t}\right]^{n-1}dx+2(T_i^{n-1}-Y_i^{n-1})=0$$

$$\text{Or}\quad K_{i+\frac{1}{2}}^{n-1}\frac{\lambda_{i+1}^{n-1}-\lambda_i^{n-1}}{\Delta x} - K_{i-\frac{1}{2}}^{n-1}\frac{\lambda_i^{n-1}-\lambda_{i-1}^{n-1}}{\Delta x}$$
$$+\frac{(C\lambda)_i^n-(C\lambda)_i^{n-1}}{\Delta t}\Delta x+2(T_i^{n-1}-Y_i^{n-1})=0$$

$$\text{Or}\quad \left(\frac{K_{i+1}^{n-1}+K_i^{n-1}}{2}\right)\frac{\lambda_{i+1}^{n-1}-\lambda_i^{n-1}}{\Delta x} - \left(\frac{K_i^{n-1}+K_{i-1}^{n-1}}{2}\right)\frac{\lambda_i^{n-1}-\lambda_{i-1}^{n-1}}{\Delta x}$$

$$\frac{(C\lambda)_i^n-(C\lambda)_i^{n-1}}{\Delta t}\,\Delta x + 2(T_i^{n-1}-Y_i^{n-1}) = 0$$

$$\text{Or}\quad -\left(\frac{K_{i+1}^{n-1}+K_i^{n-1}}{2\Delta x}\right)\lambda_{i+1}^{n-1} + \left(\frac{K_{i+1}^{n-1}+2K_i^{n-1}+K_{i-1}^{n-1}}{2\Delta x}+\frac{C_i^{n-1}\Delta x}{\Delta t}\right)\lambda_i^{n-1}$$

$$-\left(\frac{K_i^{n-1}+K_{i-1}^{n-1}}{2\Delta x}\right)\lambda_{i-1}^{n-1} = \frac{(C\lambda)_i^n}{\Delta t}\,\Delta x + 2(T_i^{n-1}-Y_i^{n-1}) \tag{A.4}$$

In this case, $n-1$ th time level is assumed to be the unknown state. The reason is that the final conditions are known for the adjoint problem and time marching proceeds from $t = t_f$ to $t = 0$.

The same control volume approach has been applied to discretise the adjoint equations for the coupled problem as well.

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